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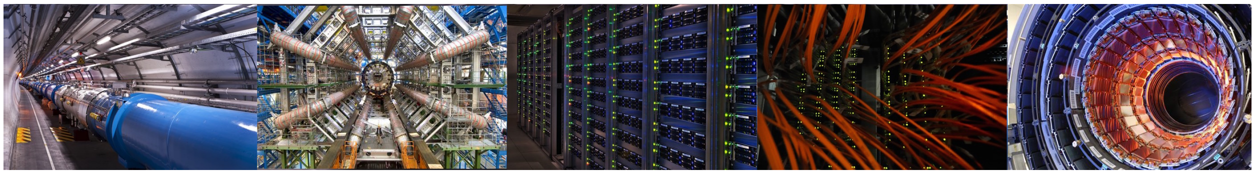

IRIS-HEP Strategic Plan for the Next Phase of Software Upgrades for HL-LHC Physics

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Editors: Brian Bockelman (Morgridge Institute), Peter Elmer (Princeton University)
Gordon Watts (University of Washington)

Contributors: Kyle Cranmer (University of Wisconsin-Madison), Matthew Feickert (University of Wisconsin-Madison), Rob Gardner (University of Chicago), Heather Gray (UC Berkeley and Lawrence Berkeley Laboratory), Alexander Held (University of Wisconsin-Madison), Daniel S. Katz (University of Illinois at Urbana-Champaign), David Lange (Princeton University), Kilian Lieret (Princeton University), Mark Neubauer (University of Illinois at Urbana-Champaign), Oksana Shadura (University of Nebraska-Lincoln), Mike Sokoloff (University of Cincinnati), Robert Tuck (Princeton University), Frank Wuerthwein (University of California, San Diego)

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Executive Summary

The quest to understand the fundamental building blocks of nature and their interactions is one of the oldest and most ambitious of human scientific endeavors. CERN's Large Hadron Collider (LHC) represents a huge step forward in this quest. The discovery of the Higgs boson, the observation of exceedingly rare decays of B mesons, and stringent constraints on many viable theories of physics beyond the Standard Model (SM) demonstrate the great scientific value of the LHC physics program. The next phase of this global scientific project will be the High-Luminosity LHC (HL-LHC) which will collect data starting circa 2029 and continue through the 2030s. The primary science goal is to search for physics beyond the SM and, should it be discovered, to study its implications. In the HL-LHC era, the ATLAS and CMS experiments will record $\sim$100 times as many collisions as were used to discover the Higgs boson (and at twice the energy). Both NSF and DOE are making large detector upgrade investments so the HL-LHC can operate in this high-rate environment. Similar investment in *software* R&D for acquiring, managing, processing and analyzing HL-LHC data is critical to maximize the return-on-investment in the upgraded accelerator and detectors.

This report presents a strategic plan for a possible second 5-year funded phase (2023 through 2028) for the **Institute for Research and Innovation in Software for High Energy Physics (IRIS-HEP)** [1, 2] which will close remaining software and computing gaps to deliver HL-LHC science. IRIS-HEP was originally funded by the NSF in September 2018 and its current funding extends through August 2023. IRIS-HEP was the result of an international community planning process in 2016-2017 that prepared a roadmap for HEP software R&D in the 2020s [3] as well as the original strategic plan [4] for how an NSF-funded Software Institute for High Energy Physics (HEP) could play a key role in meeting HL-LHC challenges. The mission of IRIS-HEP is two-fold: to serve as an active center for software R&D *and* as an intellectual hub for the larger community software R&D effort required to ensure the success of the HL-LHC scientific program. The ensemble of its activities are meant to bridge 4 key gaps to that success: (G1) raw resource gaps, (G2) scalability of the distributed computing cyberinfrastructure, (G3) executing analyses at the HL-LHC scale and (G4) sustainability of the software and computing system through the lifetime of the HL-LHC and beyond.

Building on its successes over the past 5 years, and informed by recent community workshops, IRIS-HEP will continue to pursue several high-impact R&D areas identified as those required to close those gaps and enable HL-LHC science: (1) development of highly performant analysis systems that reduce 'time-to-insight' and maximize the HL-LHC physics potential; (2) development of advanced innovative algorithms for data reconstruction and triggering; (3) development of data organization, management and access systems for the Exabyte era; and (4) facilities R&D to support the evolving requirements of the other R&D areas. A potentially important emerging opportunity, (5) Translational AI, has also been identified. IRIS-HEP will sustain the investments in the fabric for (6) distributed high-throughput computing which provides the LHC community's cyberinfrastructure with a route to the HL-LHC. Specific goals and objectives for these areas of activity include:

1. **Analysis Systems**: Modernize and evolve tools and techniques for analysis of HL-LHC data sets. The Analysis Systems area will concentrate on *G3 (Analysis at scale)* topics of managing order-of-magnitude larger data sets, enabling more complex techniques including use of modern machine learning, and the adoption of data science tools toward *G4 (Sustainability)* goals. Deliverables will include the tools supporting a full pipeline for distributed columnar data analysis at scale that are interoperable with other elements of the HEP and broader data science ecosystems. Modern machine learning techniques and operations, including differentiable analysis pipelines, will be integrated, as well as full support for analysis preservation and reinterpretation.

2. **Reconstruction and Trigger Algorithms**: Develop and evolve pattern-recognition software able to exploit next-generation detector technologies, computing platforms, and programming techniques to accurately and efficiently identify charged particle trajectories. Efforts in this area are key to eliminating *G1 (resource)* gaps due to new, and more capable, experimental apparatus, larger data rates, and evolving computing hardware. Algorithms must be engineered to be adequately *G4 (sustainable)* over the course of HL-LHC operations. This area will deliver critical components of the tracking pipeline, prioritizing algorithmic interoperability, achieving high levels of parallelism, and implementing robust algorithms. Both traditional and novel approaches to tracking algorithms will be considered as tracking is a multifaceted problem and has optimization points that vary depending on the experimental apparatus design and computing technical design.

3. **Translational AI**: Exploit Machine Learning approaches to improve the physics reach of the HL-LHC. The Translational AI area will leverage fundamental research, such as the work done by the NSF AI Institutes, and focus on helping the HL-LHC experiments translate these capabilities into production. Activities include working to enable and use ML-based services, helping the field connect to available infrastructure, and working on enabling the "retraining" of in-use models for new data.

4. **Data Organization, Management, and Access (DOMA)**: Scale and modernize the bulk data transfer infrastructure including new authorization schemes, transfer protocols, and network integration; provide new data delivery services and techniques for use in analysis facilities. DOMA contributes to the *G2 (Scalability)* computing gap to close the 20x difference in the wide-area data rates expected between now and the start of the HL-LHC. DOMA innovates new authorization schemes for inter-site bulk data transfer coordinates international data challenges to mark progress toward the target data rates and integrate new technologies. For analysis, DOMA will develop services to deliver columnar data and to provide modern data management techniques from the database community to HL-LHC analysis environments.

5. **Facilities R&D**: Innovates new approaches to building facilities for the U.S. LHC and aligns the community with approaches in the larger NSF coordinated cyberinfrastructure. The area works with Kubernetes as a "substrate" to orchestrate portable services, provides testbed facilities to projects within the Institute, and investigates the use of multi-site Kubernetes clusters to provide agility to the operation of distributed services. Facilities R&D contributes to the *G4 (Sustainability)* goal by reducing the operational complexity and costs and to *G3 (Analysis at scale)* by applying agile techniques for future analysis facilities.

6. **Fabric of distributed high-throughput computing services (OSG)**: Operates a fabric of services specifically to meet the needs of the LHC and provides a stable route to their evolution for the HL-LHC. The OSG-LHC group ensures the needs of the LHC experiments while making contributions to the larger consortium, allowing the LHC to benefit from broader common services as well.

7. **Training, Workforce Development, and Outreach**: Executes and coordinates a broad range of events to help with the training, workforce development, and outreach needs of the HL-LHC community. The area in the Institute will ensure there is training available at multiple levels of need (undergraduate, graduate, postdoc, professional) and will run the IRIS-HEP Fellows program, a in-depth virtual mentoring program targeting senior undergraduates and junior graduate students. This is key to bridging the *G4 (Sustainability)* gap.

IRIS-HEP will continue to use the concept of a "Grand Challenge" to focus activities on long-term, large-scale goals as part of the institute's overall vision. A Grand Challenge differs from a more traditional milestone or deliverable by its scale (often requiring cross-cutting teams working together), a multi-year timeframe, and the fact the entirety of the approach may not be known upfront. The challenges are executed through a series of increasingly difficult exercises coordinated throughout the community. The currently defined and planned grand challenges are:

- **Analysis Grand Challenge (AGC)**: The AGC aims to execute realistic analyses at the scale and complexity envisioned by the HL-LHC using a set of tools, facilities, and services developed within IRIS-HEP as exemplars. The AGC team coordinates an annual workshop to demonstrate current progress against the goals and to update the vision and approach as necessary.
- **Data Grand Challenge (DGC)**: The DGC for IRIS-HEP is realized as a set of global data challenges coordinated with the WLCG. These challenges, occurring biennially, bring the entire global community together to demonstrate aggregate transfer data rates and compare what is currently achievable with the HL-LHC roadmap. These challenges also provide an opportunity for integrating new technologies being worked on by DOMA into the production infrastructure.
- **Training Grand Challenge (TGC)**: To tackle the challenges of the HL-LHC, we need a workforce with broad software knowledge, spanning from basic programming skills to highly specialized training. The TGC defines a roadmap to efficiently scale up training activities and provide adequate training to create the software-skilled workforce that will realize HL-LHC science.

Additional Institute activities, such as data reconstruction and tracking, are more naturally coordinated by each experiment. IRIS-HEP will work with the experiments to integrate those deliverables with their timelines and production codes. Building on the successful R&D efforts of the first five years of the project, the second phase of IRIS-HEP will develop production-quality tools, facilities, and services that the experiments will be able to rely on for their science programs.

Lastly, as an intellectual hub, the Institute will continue to lead efforts to (1) bring together the IRIS-HEP team, key stakeholders and relevant domain experts to inform the Institute's mission, (2) bring together U.S. and international R&D efforts in "blueprint" workshops to ensure full alignment of the various efforts (3) develop partnerships between HEP and the cyberinfrastructure, computer science, and data science communities for novel approaches to meeting HL-LHC challenges, (4) bring in new effort from U.S. universities emphasizing professional development and training, and (5) sustain HEP software and underlying algorithmic and implementation knowledge over the two decades required. HEP is a global, complex, scientific endeavor. These activities will ensure that the software developed and deployed by a globally distributed community will extend the science reach of the HL-LHC and will be sustained over its lifetime.

The strategic plan targeting HL-LHC physics presented in this report for the period 2023-2028 reflects a community vision. It builds on the original planning activities in 2016-2017 and is informed by ongoing IRIS-HEP activities which engage the community including a dedicated series of workshops and conferences. The plan complements and is aligned with the experiments' HL-LHC planning activities [5–7]. IRIS-HEP is ready to deliver the software required to enable best possible HL-LHC science.

Endorsers

This strategic plan has been explicitly endorsed by ATLAS and CMS experiment representatives, as well as representatives from the US-ATLAS and US-CMS Operations programs. Specific endorsers include: Wolfgang Adam (HEPHY Vienna), Lothar Bauerdick (Fermilab), Brian Bockelman (Morgridge Institute for Research), Tulika Bose (University of Wisconsin-Madison), Kenneth Bloom (University of Nebraska-Lincoln), Paolo Calafiura (Lawrence Berkeley National Laboratory), Kyle Cranmer (University of Wisconsin - Madison), Alessandro Di Girolamo (CERN), Peter Elmer (Princeton University), Matthew Feickert (University of Wisconsin - Madison), Robert Gardner (University of Chicago), Heather Gray (University of California, Berkeley and Lawrence Berkeley National Laboratory), Oliver Gutsche (Fermilab), Alexander Held (University of Wisconsin - Madison), Michael Hildreth (University of Notre Dame), Daniel S. Katz (University of Illinois at Urbana-Champaign), Patrick Koppenburg (Nikhef), David Lange (Princeton University), James Letts (University of California, San Diego), Kilian Lieret (Princeton University), Carlos Maltzahn (University of California, Santa Cruz), Zachary Marshall (Lawrence Berkeley National Laboratory), Verena Martinez Outschoorn (University of Massachusetts Amherst), Patricia McBride (FNAL), Shawn McKee (University of Michigan), Mark S Neubauer (University of Illinois at Urbana-Champaign), Ianna Osborne (Princeton University), Danilo Piparo (CERN), Eduardo Rodrigues (University of Liverpool), Elizabeth Sexton-Kennedy (Fermilab), Oksana Shadura (University of Nebraska-Lincoln), Lucia Silvestris (INFN-Bari), Michael D Sokoloff (University of Cincinnati), Matevž Tadel (University of California, San Diego), Lauren Tompkins (Stanford University), Robert Tuck (Princeton University), Vassil Vassilev (Princeton University), Gordon Watts (University of Washington), Derek Weitzel (University of Nebraska-Lincoln), Mike Williams (MIT), Peter Wittich (Cornell University), Frank Wuerthwein (University of California, San Diego) and Avi Yagil (University of California, San Diego).

Document revisions

The revision history is:

19 December 2022 Version 0.9 - Initial draft of the document circulated for feedback and endorsements.

23 January 2023 Version 0.95 - Improved version of the document based on feedback and endorsements from version 0.9. More complete Executive Summary. Provisional version submitted to NSF.

2 February 2023 Version 1.0 - submitted to arXiv

Contents

1 Introduction

The High-Luminosity Large Hadron Collider (HL-LHC) is scheduled to start producing data in 2029 and extend the LHC physics program through the 2030s. Its primary science goal is to search for Beyond the Standard Model (BSM) physics and, should it be discovered, to study its implications. Although the basic constituents of ordinary matter and their interactions are extraordinarily well described by the Standard Model (SM) of particle physics, a quantum field theory built on top of simple but powerful symmetry principles, it is incomplete. For example, most of the gravitationally interacting matter in the universe does not interact via electromagnetic or strong nuclear interactions. As it produces no directly visible signals, it is called dark matter. No particles or fields of the SM can account for its existence. Equally as important, the SM does not address fundamental questions related to the detailed properties of its *own* constituent particles or the specific symmetries governing their interactions. To achieve this scientific program, the HL-LHC will record data from 100 times as many proton-proton collisions as did Run 1 of the LHC, with both more complex detectors and where each collision will be far more complex to process.

Realizing the full potential of the HL-LHC requires large investments in upgraded hardware. The construction projects for these hardware upgrades are now underway. The two general purpose detectors at the LHC, ATLAS and CMS, are operated by collaborations of more than 3000 scientists each. U.S. personnel constitute about 30% of the collaborators on these experiments. Within the U.S., funding for the construction and operation of ATLAS and CMS is jointly provided by the Department of Energy (DOE) and the National Science Foundation (NSF). Funding for U.S. participation in the LHCb experiment is provided only by the NSF. The NSF is also playing a major role in the hardware upgrade of the ATLAS and CMS detectors for the HL-LHC, through Major Research Equipment and Facilities Construction (MREFC) funding which began in 2020.

The HL-LHC **also requires a commensurate investment in software research and development** and deployment. Software is necessary to acquire, manage, process, and analyze the data. Current estimates of HL-LHC computing needs significantly exceed what will be possible – even assuming Moore's Law – with constant operational budgets [5, 6]. The underlying nature of computing hardware (processors, storage, networks) is also evolving, the quantity of data to be processed is increasing dramatically, its complexity is increasing, and more sophisticated analyses will be required to maximize the HL-LHC physics yield. The magnitude of the HL-LHC computing problems to be solved will require different approaches.

The existing computing system of the LHC experiments is the result of almost 20 years of effort and experience. In addition to addressing the significant future challenges, sustaining the fundamental aspects of what has been built to date is also critical. Fortunately, the collider nature of this physics program implies that essentially all computational challenges are "pleasantly" parallel. The large LHC collaborations each produce tens of billions of events per year through a mix of simulation and data triggers recorded by their experiments, and all events are statistically independent of each other, and can be processed in parallel. This intrinsic simplification from the science itself permits aggregation of distributed computing resources and is well-matched to the use of *high throughput computing* to meet LHC and HL-LHC computing needs. In addition, the LHC today requires more computing resources than will be provided by funding agencies in any single location (such as CERN). Thus *distributed high-throughput computing* (DHTC) will continue to be a fundamental characteristic of the HL-LHC and evolving the DHTC is essential for the HEP community.

In planning for the HL-LHC, it is critical that all parties agree on the software goals and priorities, and that the efforts tend to complement each other; for IRIS-HEP, this alignment process began in 2016 and is ongoing to this day. The process was started with a HEP Software Foundation (HSF) planning exercise in late 2016 to prepare a Community White Paper (CWP) [3] whose goal was to provide a roadmap for software R&D in preparation for the HL-LHC era. The community identified and prioritized the software research and development investments required:

1. to enable new approaches to computing and software that can radically extend the physics reach of the detectors; and
2. to achieve improvements in software efficiency, scalability, and performance, and to make use of the advances in CPU, storage, and and network technologies;
3. to ensure the long term sustainability of the software through the lifetime of the HL-LHC.

In parallel to this global exercise, and with funding from the NSF, the U.S. community executed a conceptualization process to produce a Strategic Plan for how a Scientific Software Innovation Institute (S^2I^2) for high-energy physics (HEP) could help meet the HL-LHC challenges. Specifically, the S^2I^2-HEP conceptualization process [8] had three additional goals:

1. to identify specific focus areas for R&D efforts that could be part of an S^2I^2 in the U.S. university community;
2. to build a consensus within the U.S. HEP software community for a common effort; and
3. to engage with experts from the related fields of scientific computing and software engineering to identify topics of mutual interest and build teams for collaborative work to advance the scientific interests of all the communities.

This resulted in a document, the *"Strategic Plan for a Scientific Software Innovation Institute (S^2I^2) for High Energy Physics"* [4]. In September, 2018, NSF funded the "Institute for Research and Innovation in Software for High Energy Physics (IRIS-HEP)", a collaboration of 19 U.S. universities (Figure 1), to execute a program of work to realize that strategic plan.

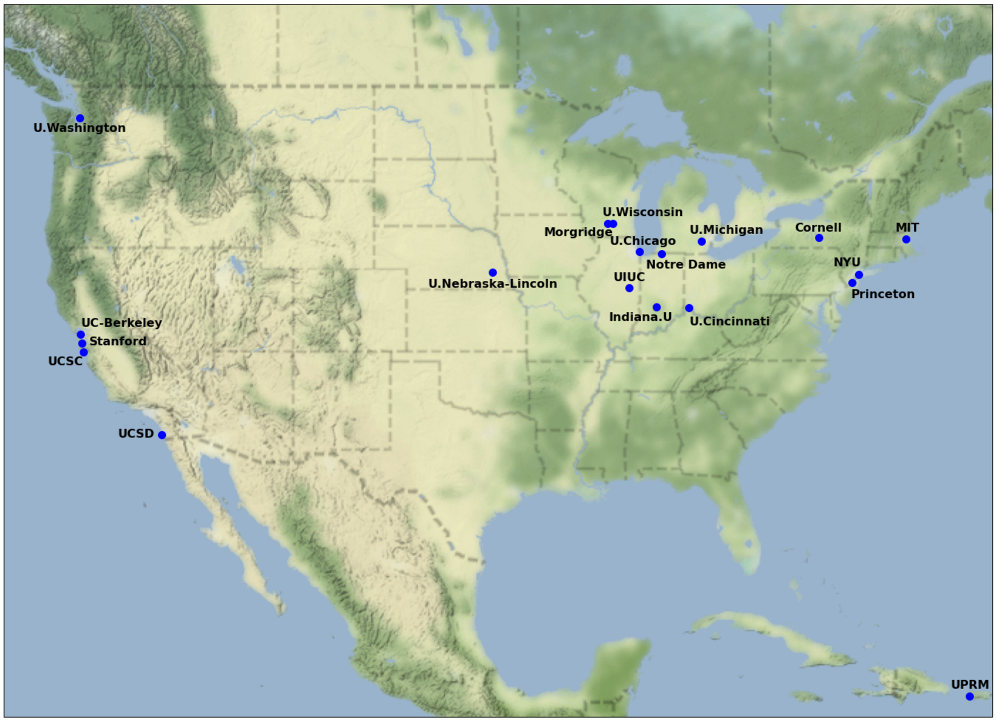

Figure 1: Institutions funded during the first phase (2018-2023) of the IRIS-HEP software institute.

IRIS-HEP also plays a primary leadership role in the international HEP community to prepare the "software upgrade" which runs in parallel to the hardware upgrades being executed for the HL-LHC. IRIS-HEP exists within a larger context of international and national projects. As an intellectual hub for software R&D, it is building a more inclusive community process for developing, prototyping, and deploying software. It drives research and development in a specific set of areas (see Section 5 for the plans for the next phase of the institute) using its own resources directly, and also leveraging them through collaborative efforts. After a two-year startup phase, IRIS-HEP began an execution phase and has the technical team, project management, and governance structures in place necessary to achieve the large-scale vision expected of an institute-class entity. Accomplishments of this phase include the construction of an analysis pipeline based on the Python Data Science ecosystem; delivery of a new, vectorized Kalman Filter algorithm into use at CMS; transitioning the LHC cyberinfrastructure to a new, HTTP-based bulk data transfer protocol; rolling out the use of a new authorization paradigm based on capability tokens; and delivering a composable, Kubernetes-based Facilities R&D platform for the community to use.

IRIS-HEP is in its fifth year. It has executed on the strategic plan laid out by the S^2I^2 conceptualization project, but has also started evolving beyond the initial conditions of the plan. Thus, the institute has led a planning process including both community planning workshops (see Appendix A) and internal exercises. This updated strategic plan is a vision for what must be accomplished in the next five years by the institute to enable HL-LHC physics.

2 Science Drivers

IRIS-HEP aims to deliver the software required for the HL-LHC science case, in particular enabling the discovery of BSM physics and the eventual study its details. To understand why discovering and elucidating BSM physics will be transformative, we need to start with the key concepts of the SM, what they explain, what they do not, and how the HL-LHC will address the latter.

In the past 200 years, physicists have discovered the basic constituents of ordinary matter and they have developed a very successful theory to describe the interactions (forces) among them. All atoms, and the molecules from which they are built, can be described in terms of these constituents. The nuclei of atoms are bound together by strong nuclear interactions. Their decays result from strong and weak nuclear interactions. Electromagnetic forces bind atoms together, and bind atoms into molecules. The electromagnetic, weak nuclear, and strong nuclear forces are described in terms of quantum field theories. The predictions of these theories are extremely precise, generally speaking, and they have been validated with equally precise experimental measurements. The electromagnetic and weak nuclear interactions are intimately related to each other, but with a fundamental difference: the particle responsible for the exchange of energy and momentum in electromagnetic interactions (the photon) is massless while the corresponding particles responsible for the exchange of energy and momentum in weak interactions (the W and Z bosons) are about 100 times more massive than the proton. A critical element of the SM is the prediction (made more than 50 years ago) that a qualitatively new type of particle, called the Higgs boson, would give mass to the W and Z bosons. Its discovery at the LHC by the ATLAS and CMS Collaborations in 2012 [9, 10] confirmed experimentally the last critical element of the SM.

The SM describes essentially all known physics very well, but its mathematical structure and some important empirical evidence tell us that it is incomplete. These observations motivate a large number of SM extensions, generally using the formalism of quantum field theory, to describe BSM physics. For example, "ordinary" matter accounts for only 5% of the mass-energy budget of the universe, while dark matter, which interacts with ordinary matter gravitationally, accounts for 27%. While we know something about dark matter at macroscopic scales, we know nothing about its microscopic, quantum nature, *except* that its particles are not found in the SM and they lack electromagnetic and SM nuclear interactions. BSM physics also addresses a key feature of the observed universe: the apparent dominance of matter over anti-matter. The fundamental processes of leptogenesis and baryongenesis (how electrons and protons, and their heavier cousins, were created in the early universe) are not explained by the SM, nor is the required level of CP violation (the asymmetry between matter and anti-matter under charge and parity conjugation). Constraints on BSM physics come from "conventional" HEP experiments plus others searching for dark matter particles either directly or indirectly.

The LHC was designed to search for the Higgs boson and for BSM physics – goals in the realm of discovery science. The ATLAS and CMS detectors are optimized to observe and measure the direct production and decay of massive particles. They are now measuring the properties of the Higgs boson more precisely to test how well they accord with SM predictions.

Whereas ATLAS and CMS were primarily designed to study high mass particles directly, LHCb was designed to study heavy flavor physics where quantum influences of very high mass particles, too massive to be directly detected at LHC, are manifest in lower energy phenomena. Its primary goal is to look for BSM physics in CP violation (CPV, defined as asymmetries in the decays of particles and their corresponding antiparticles) and rare decays of beauty and charm hadrons. As an example of how one can relate flavor physics to extensions of the SM, Isidori, Nir, and Perez [11] have considered model-independent BSM constraints from measurements of mixing and CP violation. They assume the new fields are heavier than SM fields and construct an effective theory. Then, they "analyze all realistic extensions of the SM in terms of a limited number of parameters (the coefficients of higher dimensional operators)." They determine bounds on an effective coupling strength couplings of their results is that kaon, B_d, B_s, and D^0 mixing and CPV measurements provide powerful constraints that are complementary to each other and often constrain BSM physics more powerfully than direct searches for high mass particles.

The Particle Physics Project Prioritization Panel (P5) issued their *Strategic Plan for U.S. Particle Physics* [12] in May 2014. It was very quickly endorsed by the High Energy Physics Advisory Panel and submitted to the DOE and the NSF. The report says, *we have identified five compelling lines of inquiry that show great promise for discovery over the next 10 to 20 years. These are the Science Drivers:*

- *Use the Higgs boson as a new tool for discovery*
- *Pursue the physics associated with neutrino mass*
- *Identify the new physics of dark matter*
- *Understand cosmic acceleration: dark matter and inflation*
- *Explore the unknown: new particles, interactions, and physical principles.*

The HL-LHC will address the first, third, and fifth of these using data acquired at twice the energy of Run 1 and with 100 times the luminosity. As the P5 report says,

> *The recently discovered Higgs boson is a form of matter never before observed, and it is mysterious. What principles determine its effects on other particles? How does it interact with neutrinos or with dark matter? Is there one Higgs particle or many? Is the new particle really fundamental, or is it composed of others? The Higgs boson offers a unique portal into the laws of nature, and it connects several areas of particle physics. Any small deviation in its expected properties would be a major breakthrough.*
>
> *The full discovery potential of the Higgs will be unleashed by percent-level precision studies of the Higgs properties. The measurement of these properties is a top priority in the physics program of high-energy colliders. The Large Hadron Collider (LHC) will be the first laboratory to use the Higgs boson as a tool for discovery, initially with substantial higher energy running at 14 TeV, and then with ten times more data at the High- Luminosity LHC (HL-LHC). The HL-LHC has a compelling and comprehensive program that includes essential measurements of the Higgs properties.*

Summary of Physics Motivation: The ATLAS and CMS collaborations published letters of intent to do experiments at the LHC in October 1992, about 30 years ago. At the time, the top quark had not yet been discovered; no one knew if the experiments would discover the Higgs boson, supersymmetry, technicolor, or something completely different. Looking forward, no one can say what will be discovered in the HL-LHC era. However, with data from 100 times the number of collisions recorded in Run 1 the next 20 years are likely to bring even more exciting discoveries.

3 HL-LHC Software and Computing Gaps

With the start of the HL-LHC era approximately 5 years away, the broad outlines of the remaining software capability gaps to deliver HL-LHC science have emerged. Bridging these "gaps" requires the community to maintain a robust R&D program between now and the start of the HL-LHC. This will make a direct impact on the quantity and quality of the science that can be performed.

The cyberinfrastructure requirements for HL-LHC are driven by science needs. The experiments have assessed the needs to enable the precision and discovery potential of the HL-LHC data set based on extensive simulation analyses [13–15]. These analyses probed the capabilities of the upgraded detectors, the potential of 3000 fb^{-1} datasets, and requirements driven by the increased event complexity that comes with the much higher luminosity of HL-LHC. One important outcome of these studies were estimates for the needed event rates into the online trigger and the offline computing facilities of the experiment. While these estimates, particularly the offline ones, are still evolving as LHC data analysis continues, they serve as the baseline for defining the overall cyberinfrastructure needs for HL-LHC.

HL-LHC Software and Computing Gaps

The four software and computing gaps discussed at length in this section are:

G1. **Raw resource gaps**: The HL-LHC dataset will be enormous. Event complexity and count will each go up by about an order of magnitude. If no improvements to algorithms or resource management techniques are made, the HL-LHC experiments will simply be unable to process and store the data necessary for the science program.

G2. **Scalability of the distributed computing cyberinfrastructure**: It is insufficient to buy cores and disk alone – the cyberinfrastructure used by the experiments must also scale to support the volume of hardware. This challenge is especially acute when it comes to data transfers: both the software must be ready and the shared networking resources (e.g., ESNet in the US) must be appropriately managed.

G3. **Analysis at scale**: Analysis at the HL-LHC will be markedly different for two reasons: (a) the scale of the datasets involved and (b) the use of next-generation techniques (such as the latest machine learning techniques) to increase the scientific reach of each result. The former will require users to heavily utilize dedicated 'analysis facilities', optimized for high data rate I/O and the latter will require new services and data management techniques to be developed.

G4. **Sustainability**: HEP is a facilities-driven science - the cyberinfrastructure assembled for an experiment must last or evolve on the decadal scale. This limits some strategies to cyberinfrastructure - for example, it is impossible for LHC to "do it yourself" and own the entire software stack. Specific sustainability strategies must be implemented even at the R&D phase to ensure that the cyberinfrastructure put in place at the beginning of the experiment is one the community can afford.

3.1 Raw Resource Gaps

Even before Run 1 started in 2009, a dedicated scrutiny group annually reviewed the raw resource requests from the LHC experiments. The input to these projections come from a few physics inputs (planned seconds of the LHC runtime, physics events recorded per second, average luminosity) and technical inputs (average size of event, simulation time per event, reconstruction time per event);

Parameter	Run 3 (2022-2025)	Run 4 (2029-2032)	Run 5 (2035-2037)
LHC Energy [TeV]	13.6	14.0	14.0
Average pileup	50	140	200
Running time [Msec/year]	6	6	6
Integrated luminosity [fb^{-1}/year]	80	270	350

Table 1: Summary of the expected data volumes collected by ATLAS and CMS during a typical year of LHC Run 3 and during the HL-LHC program.

combined with an experiment's computing model, guidance for the aggregate CPU, disk, and tape needs were produced for the next three years.

Similarly, starting in about 2016, the community has provided predictions about the resource needs for HL-LHC. These estimates have larger uncertainties - it is unclear what performance gains R&D will provide the community and the expected compute purchasing power a decade out - but have helped the community to understand potential resource gaps.

Background: The HL-LHC computing infrastructure must provide sufficient raw resources in order to carry out the science programs of the HL-LHC experiments. There are two aspects where commodity hardware is used at large scale: the online system includes a large compute facility to select events using a software-based trigger; and the offline system, which is responsible for carrying out numerous tasks including data processing, simulation production and analysis. These cyberinfrastructure needs are typically tracked in terms of compute (CPU, GPU, etc), rapid access storage (disk), long-term storage (tape), and wide-area network needs. Experiments regularly estimate compute requirements for both the long term (next 5-10 years) and short term (next 1-3 years) based upon their understanding of what resources will be needed to support the HL-LHC scientific program. Focusing on the US university program, we discuss primarily the compute and disk storage requirements of the offline computing system.

The same basic approach is used by the experiments to derive both short and long term resource projections. The approach is simply to start from today's computing model and operational plan from the accelerator and fold in research and development outcomes that will reduce (or rarely increase) the required computational resources in the future. These estimates include models for data processing, needs for simulation production, analysis processing and data management. Projections have numerous sources of uncertainty, including the LHC schedule, the changes in the scope of the physics program as LHC results progress, as well as evolution in software performance due to on-going R&D. Naturally, these are substantially larger in the long term projections.

As a means of comparison, these resource needs are compared with projections of the distributed computing infrastructure in place given assumptions about future budgets, or alternatively simply the percentage by which resources will increase each year. Just as the model projections are uncertain, the resource projections are uncertain given variations in technology evolution and market forces. Combined, the compute requirements and resource projections gives guidance on the potential raw resource gap.

Resource Projections: Figure 2 shows ATLAS and CMS projections for CPU and disk needs through the first two running periods of the HL-LHC program. As summarized in Table 3.1, Run 4 (starting 2029) is expected to have up to 140 simultaneous pp interactions during each bunch crossing (each 25 ns), while Run 5 is expected to have up to 200 such interactions. The integrated luminosity during this period is expected to be up to 350 fb^{-1}. During Run 4, the ATLAS experiment currently expects around 10 kHz of events entering the offline system, while

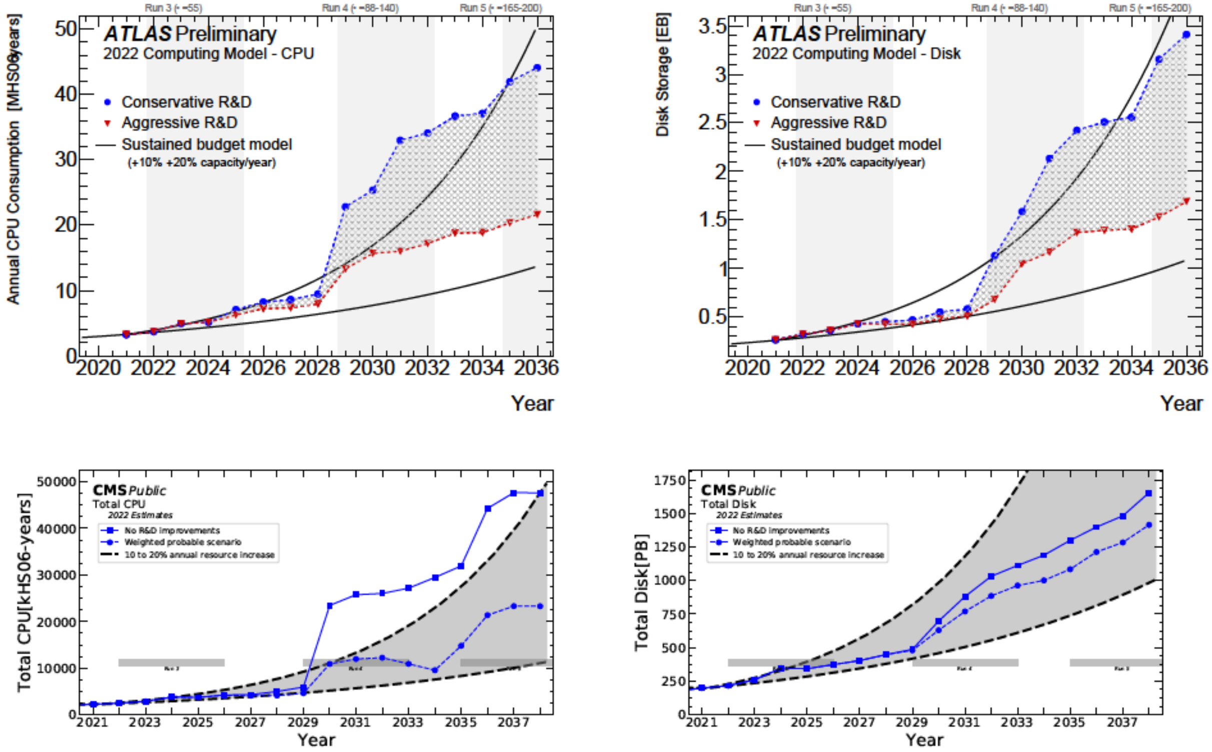

Figure 2: Current Atlas (top) and CMS (bottom) projections for CPU (left) and disk (right) requirement evolution through the first two data taking runs of HL-LHC. Each projection includes baseline estimates, and estimates including improvements that can be achieved through R&D between now and the start of HL-LHC. Each experiment has published detailed documents [5, 6] on these projections for a LHCC recent review [16].

CMS around 5 kHz. These can be compared to around 5 kHz of data collected by each experiment during the 2022 run. In each case, the full raw is kept for all of these events.

Experiments have also started to incorporate the impact of future R&D outcomes on their resource projections. For example, the adoption of small, columnar, data formats for analysis can substantially reduce the disk requirements of an experiment. Similarly, a speed up in event reconstruction application timing will reduce the compute requirements. As R&D outcomes are naturally uncertain, extrapolations are done with different assumptions of what is most likely to be realized from ongoing research. Projections are generally conservative in this regard, as developers typically realize gains in performance not anticipated years in advance of their research.

The other primary uncertainty component is driven by the needs of the HL-LHC physics program. The experiments have gained substantial knowledge during Run 2 which has lead to a broadened science program during Run 3. In particular, both CMS and ATLAS have substantial datasets for b-physics studies that were not included in the HL-LHC projections for event rates made in the mid-2010s. This was made possible by continued emphasis on performance optimization to reduce resource needs. We anticipate that the experiments will continue to refine their needs for HL-LHC as the LHC Run 3 program (which has just completed its first year of operations) progresses.

Bridging the Resource Gap

IRIS-HEP will continue to develop advanced reconstruction and trigger algorithms (Section 5.2), with a particular emphasis on charged particle tracking. It will also invest in an emerging area, Translational AI (Section 5.3), with significant potential.

3.2 Scalability of the overall distributed computing cyberinfrastructure

While the HL-LHC experiments have not yet completed their technical design reports, they are expected to utilize the successful distributed computing-based approach of the LHC. Distributed cyberinfrastructure provides flexibility in placement of resources and allows the community to take advantage of opportunities such as new resources wherever they may be. It also helps the infrastructure scale as no single site needs to be large enough to support a single experiment.

One tradeoff of the distributed approach is the higher reliance on middleware and wide-area network (WAN) services. While parts of the global LHC community have dedicated network paths solely for the experiments, in the US most facilities heavily utilize the shared ESNet fabric. ESNet provides connectivity for site-to-site transfers within the US and the transatlantic connectivity to CERN.

The *scalability* challenge for the HL-LHC largely revolves around scaling up data rates for this shared resource, demonstrating this capability, and ensuring the network providers have sufficient tooling to monitor and manage HL-LHC traffic. This is an area where purchasing hardware is not enough - the entire stack, including file transfer software, must be tuned and prepared for the challenge.

From the raw resource requirements for the HL-LHC, one can derive reasonable estimates of the WAN data rates that must be sustained (e.g., if hypothetically 100PB of raw data taken at CERN is assigned to Fermilab to process in the last three months of the year, we know at least 110Gbps sustained for 90 days is necessary to move the inputs). As of 2021, the Worldwide LHC Computing Grid (WLCG) [17] estimates the worldwide set of facilities will need to transfer at an aggregate of 10Tbps for HL-LHC, including 900Gbps to Brookhaven National Laboratory, 1.6Tbps to Fermi National Accelerator Laboratory, and 2,500 across the transatlantic link. In 2021, ESNet ran a requirements review [18] that estimated a nominal Tier-2 site would need 400Gbps of connectivity at the startup of HL-LHC. These numbers are approximately 20x larger than what is done today.

To meet these scalability requirements, the community has defined the Data Grand Challenge (Section 6.2) as a series of escalating biennial exercises that culminate in 2025 at 100% of the expected HL-LHC data transfer scale. The Data Organization, Management, and Access (DOMA) strategic area has defined a complementary sequence of work that uses the data challenges as a periodic integration point where progress against the goal can be measured.

The Data Grand Challenge helps prepare the cyberinfrastructure for the scalability challenge in data movement. Another aspect of the scalability challenge is the computing middleware - acquiring all the disparate resources into a virtual resource pool and executing scientific workflows (data reconstruction, simulation, analysis dataset derivation). These managed compute resources will also grow by an order of magnitude. However, the compute scalability challenge is more modest as some of the resource growth is canceled out by the increase in parallelism of each compute tasks, meaning the number of overall running tasks remains roughly the same order of magnitude. For compute, the experiments share a common software layer of “Compute Entrypoints” (CEs) used to submit “pilot” jobs that acquire capacity from remote batch systems. The OSG-LHC group helps to manage the CE and other distributed middleware running on U.S. LHC computing facilities.

Because the scalability of the CI affects how many distributed computing resources are available to HL-LHC experiments, meeting this challenge is directly related to the HL-LHC science goals:

without input data moved to the processing location and the ability to process at scale, HL-LHC science cannot be performed!

Bridging the Cyberinfrastructure Scalability Gap

Many Data Organization, Management and Organization (DOMA) activities in IRIS-HEP (Section 5.4) are designed to help scale bulk data transfer and bridge this gap. A dedicated Data Grand Challenge (Section 6.2) activity will work with the community to measure progress and deliver for HL-LHC.

3.3 Analysis at scale

A physics analysis in the HL-LHC era will be more than 10 times larger than a Run 1- or 2-era physics analysis as measured by event count alone. New techniques increasing physics sensitivity and controlling systematic errors will be more important in HL-LHC physics analyses. Technologies which empower smaller, more agile analysis teams will be required to do the breadth of science expected at the HL-LHC and to democratize participation across the collaborations. The analysis model must thus change to fulfill the HL-LHC physics program.

Analysis refers to the final stage of the physics pipeline - taking official datasets produced by an experiment and turning them into published scientific results and discoveries. This means spinning through the data to build histograms and other aggregated quantities. In Run 1 and 2, the largest analysis datasets are 100's to 10,000's of gigabyte. In the HL-LHC they will regularly range into 100's to 1,000's of *terabytes* in size. Three aspects of the way our community performs this work as shown in Figure 3 are not sustainable in the HL-LHC era. First, the intermediate datasets that are produced for each analysis or group of analyses, largely containing copies of the official data, will take up ever-larger amounts of disk resources that will no longer be within budget. Second, creating derivative datasets from the official data takes 1-2 weeks with current approaches. Scaling these costs by the 10x additional data, a new idea that requires new data, selection cuts, or new datasets would require months. Innovation and leading-edge science becomes prohibitively expensive for students. Third, there is not enough automation to support smaller analysis teams. Processing this data at scale, in a timely manner, will involve novel methods of data delivery and distributed processing; where small clusters and sometimes even laptops are enough for HL-LHC, a larger 'analysis facility' with advanced supporting services will be necessary.

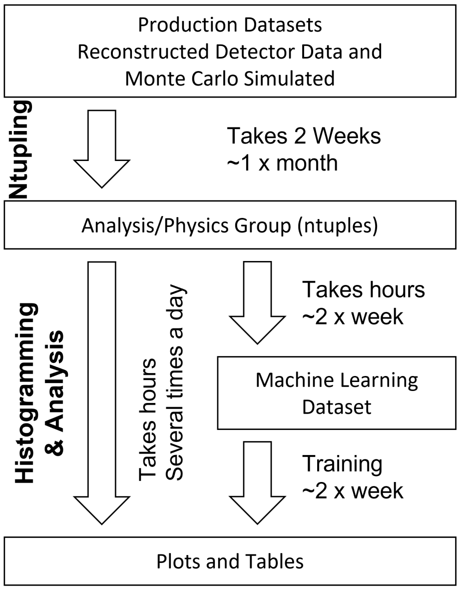

Figure 3: Data and Analysis workflow for a traditional Run 2 and Run 3 physics analysis at the LHC.

Different types of physics analyses use different tools and have different data access patterns. The ATLAS and CMS experiments have published papers detailing some of the important physics analyses for the HL-LHC [15] and attempting to quantify how much data is needed and the expected physics reach for the HL-LHC. From this, we highlight three analyses that can be used as flagships or exemplars through the next phase of IRIS-HEP to illustrate our tools and approaches:

- **High-volume**: An example physics analysis that will require extremely large datasets is the top quark mass measurement in the $t\bar{t} \rightarrow 1 + \text{jets}$ channel. The large backgrounds in this analysis channel mean the best acceptance occurs with the largest dataset. The backgrounds are modeled with Monte Carlo simulation, which makes for very large simulated datasets. This is a prototypical high-volume analysis.

- **High-complexity**: Di-Higgs measurements probe the Higgs self coupling, which allow us to probe the source of Electro-Weak Symmetry Breaking - which underlies the recently discovered Higgs mechanism. This is one of the flagship measurements for the HL-LHC. Even with the full dataset from the HL-LHC, the sensitivity to the Higgs self-coupling is just barely possible. This is a good example of an analysis that will need every tool to improve its sensitivity; Machine Learning and the use of many control regions to control systematics are some examples.
- **Baseline**: Finally, a $t\bar{t}$ cross section measurement is a well understood and easily reproduced measurement. There is also Open Data available now on which scale tests can be run.

Analysis at scale requires many individual tools to work together. IRIS-HEP and the community created the Analysis Grand Challenge (AGC) to integrate across the Analysis Systems, DOMA, and Facilities R&D areas and to demonstrate progress toward the HL-LHC goals; it is the mechanism IRIS-HEP will use to show the analysis at scale gap is closing. The AGC uses modern tools built by Analysis Systems, data delivery, and prototype analysis facilities to perform all steps of a physics analysis. This includes initial reading of the datasets, building histograms, determining statistical and systematic errors, performing the statistical analysis, and, finally, producing the plots for the paper that contains the physics results. In the current phase of IRIS-HEP, AGC uses CMS Open Data and partially implements the **baseline** $t\bar{t}$ cross section measurement. Over the next phase, the Institute can demonstrate it is closing the gap by expanding the baseline and implementing a realistic **high-volume** Higgs self-coupling measurement and a **high-complexity** $t\bar{t}$ top mass measurement.

Bridging the Analysis at Scale Gap

The Analysis Systems activities in IRIS-HEP (Section 5.1) develop many key software elements to bridge this gap, while leveraging DOMA (Section 5.4) projects which enable efficient data delivery to analysis. The Analysis Grand Challenge (Section 6.1) is designed to work with the community to integrate the full system and demonstrate the scale required for HL-LHC.

3.4 Sustainability

The long term sustainability of the software ecosystem is critical for HEP, given that the HL-LHC and other facilities of the 2020s will be relevant through at least the 2030s. Key components of 'scalability' include improved adaptability to new challenges, software longevity, and efficiency. We aim to ensure that the software will be easier to develop and maintain so that it remains available in the future on new platforms, meets new needs, and is as reusable as possible. Sustainability is also closely connected to the available workforce; a balance is needed between the continuity of individuals – as active effort or intellectually – through the desired sustainability period and the need to attract and integrate new people over time. The LHC community is **in danger of a sustainability gap** in the HL-LHC era: care must be taken to ensure we don't have more software than we can sustain with the workforce we will have during the HL-LHC program.

Over the past few years, IRIS-HEP has been working with the community [19, 20] to improve software sustainability through increased intentionality around how and what software is developed. The specific activities are centered both *(a)* on defining and evolving the software ecosystem and *(b)* workforce development.

Software Ecosystem: As a facilities-based science and with computing playing a key role within the facility, one can expect that some limited amount of "operations" effort will be associated to computing needs for the lifetime of the facility, but clear strategic choices need to be made to ensure the cyberinfrastructure is manageable within the operational effort. Given the nature of the current LHC and HEP software ecosystem, two paths are particularly relevant:

- **Identification and consolidation of redundant HEP-specific solutions:** For a number of historical and organizational reasons, many HEP software solutions are developed within the context of single experiments. In cases where the experiments actually have similar needs, this has led to multiple solutions to the same problem.
- **Adoption of solutions used by a wider scientific or open source community:** By moving to more widely used solutions the base of support for sustainability issues typically also becomes larger.

Both of these paths effectively boil down to increasing the size of the community using a given software element. Most software products cannot survive and thrive without *some* level of dedicated effort and "ownership" by some institution or long running project. In cases where increasing the size of the community does not significantly increase the scope of the software, the increase effectively increases the impact of effort invested. Concentrating available community effort on a single solution will ultimately lead to better, more sustainable solutions.

For example, instead of maintaining standalone distributed high-throughput computing services within the Institute, IRIS-HEP's OSG-LHC team 5.6 contributes to the larger OSG Consortium. In this way, common services needed can be shared across the NSF Science and Engineering, greatly reducing the total effort needed in this area.

While some software has been delivered for LHC Run 3, efforts to conslidate and leverage must continue until software solutions and computing systems are deployed for HL-LHC. This focus on sustainability is integrated into all of the Institute activities, and the choices we make, described in Sec. 5.

Workforce Development and Evolution: People are also key to software sustainability. The Training activities of IRIS-HEP (Section 5.7) are central elements for working with the community to develop more sustainable software practices and skills from the ground up. The Institute's Blueprint activity aims to build community consensus around more sustainable choices and activities.

The Institute plays a driving role in particular for the earlier stages of the software lifecycle. It then partners with other organizations (the experiments, the US LHC operations programs, specific institutions) for the later elements of the lifecycle and to develop sustainability paths for for the long run.

Finally, we note that **cross-disciplinary and broadly used software with a self-supporting community democratizes science, eliminating the need for specialized technical knowledge** and enabling researchers to gain equal access to help.

Bridging the Sustainability Gap

Engineering for sustainability is built into all IRIS-HEP software activities. Strategically, IRIS-HEP Analysis Systems (Section 5.1) activities are enabling the adoption of more broadly used data science tools. DOMA activities 5.4 work to deliver common software tools across HEP. Most importantly, the IRIS-HEP Training activities 5.7 and the Training Grand Challenge 6.3 are leading the community to prepare the workforce for the HL-LHC era.

4 The Institute Role

4.1 Institute Role within the HL-LHC Community

The mission of IRIS-HEP is to execute directly a set of R&D activities and to serve as an intellectual hub for the larger community R&D effort required to close the HL-LHC Computing Gaps. The timeline for the LHC and HL-LHC is shown in Figure 4; a 2nd phase for IRIS-HEP will operate roughly in the 5 year period from 2023 to 2028, after the end of funding for IRIS-HEP through the end of the R&D window before HL-LHC starts in 2029. This time period will coincide with two important steps in the ramp up to the HL-LHC: the delivery of the Computing Technical Design Reports (CTDRs) by the ATLAS and CMS experiments in ∼2025 and Long Shutdown 3 in 2026-2028. The CTDRs will describe the experiments' technical blueprints for building software and computing to maximize the HL-LHC physics reach, given the financial constraints defined by the funding agencies. For ATLAS and CMS, the increased size of the Run 3 data sets relative to Run 2 are not expected to be a major challenge, and changes to the detectors will be modest compared to the upgrades anticipated for Run 4. As a result, ATLAS and CMS have an opportunity to continue prototyping and deploying some elements of HL-LHC computing during Run 3, particularly during the end of year technical shutdowns, and to perform infrastructure scaling tests alongside the production workloads. In contrast, LHCb made a major transition in terms of how much data will be processed at the onset of Run 3 and HL-LHC will be a smaller change; in the next phase of IRIS-HEP, the team would start working on early research necessary for Run 5.

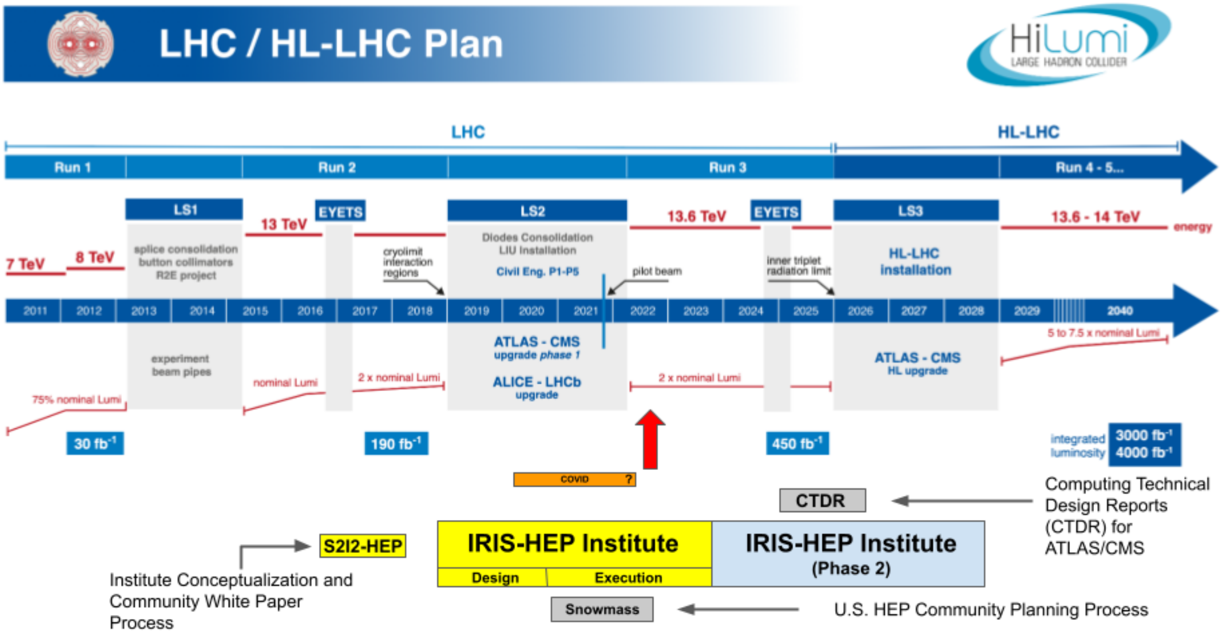

Figure 4: Timeline for the LHC and HL-LHC [21] as of January 2022, indicating both data-taking periods and "shutdown" periods which are used for upgrades of the accelerator and detectors. Data-taking periods are indicated by the (lower) red lines showing the relative luminosity and (upper) red lines showing the center of mass energy. Shutdowns with no data-taking are indicated by blue boxes (LS = Long Shutdown, EYETS = Extended Year End Technical Stop). The planning and award periods for the current IRIS-HEP award are shown in yellow.

IRIS-HEP exists within a larger context of international and national projects that are required for software and computing to successfully enable science at the LHC, both today, and in the future. Most importantly at the national level, this includes the U.S. LHC "Operations Programs," jointly funded by DOE and NSF, as well as the OSG Consortium. At the international level, important partners include both the HEP Software Foundation (HSF) and the Worldwide LHC Computing Grid (WLCG). Both international organizations serve primarily as coordination and consensus-building bodies and are helpful for projects like IRIS-HEP that want to communicate across the entire field. HSF focuses primarily on physics software whereas WLCG coordinates the facilities, middleware, and operations of the global production infrastructure.

The Institute's mission is through cooperative, community process for developing, prototyping, and deploying software. A strength of an institute-scale approach is that it becomes greater than the sum of its parts, and the larger community efforts it engenders produce better and more sustainable software than would be possible otherwise. Consistent with this mission, the role of IRIS-HEP is to:

1. Drive the software R&D process in specific focus areas using its own resources directly, and also leveraging them through collaborative efforts (see Section 5).

2. Work closely with the LHC experiments, their U.S. Operations Programs, the relevant national laboratories, and the larger HEP community to identify the highest priority software and computing issues and then create collaborative mechanisms to address them.

3. Serve as an intellectual hub for the larger community effort in HEP software and computing. IRIS-HEP brings together a critical mass of experts from HEP, other domain sciences, academic computer science, and the private sector to advise the HEP community on sustainable software development. Similarly, the Institute serves as a center for disseminating knowledge related to the current software and computing landscape, emerging technologies, and tools. It will continue to provide critical evaluation of new proposed software elements for algorithm essence (e.g. to avoid redundant efforts), feasibility and sustainability, and provide recommendations to collaborations (both experiment and theory) on training, workforce, and software development.

4. Deliver value through its (a) contributions to the development of the CTDRs for ATLAS and CMS and (b) research, development and deployment of software and services.

4.2 The Institute as an Intellectual Hub

One highly successful aspect of the IRIS-HEP – reinforcing the value of the institute structure itself – is its role as an intellectual hub for the broader community. Through a series of organized activities, IRIS-HEP brings together the entire HEP community (even beyond the Institute's science driver of HL-LHC) to work on specific problems, disseminate knowledge and share experience.

Through this community Intellectual Hub role, IRIS-HEP is able to directly impact experiments such as DUNE, EIC, Belle II, FCC, SPT-3G, XenonNT, and NoVA via its physics software, trainings, and shared cyberinfrastructure. For example, the analysis tools projects and ACTS are being evaluated and utilized by EIC, Belle II, and FCC. The services (particularly, the software stack) produced by the OSG-LHC are incredibly popular within the HEP community; not only are these used by DUNE, SPT-3G, XenonNT, and NoVA but by almost every large HEP collaboration within the US. As part of this Intellectual Hub component, the Institute will help coalesce and guide the broader HEP community.

Specific activities done as part of the Intellectual Hub are the *Blueprint Activity* and running the series of *Coordinated Ecosystem Workshops*:

- **Blueprint Activity**: The IRIS-HEP Blueprint activity is designed to inform development and evolution of the IRIS-HEP strategic vision and build (or strengthen) partnerships among communities driven by innovation in software and computing. The blueprint process includes a series of workshops that bring together IRIS-HEP team members, key stakeholders, and domain experts from disciplines of importance to the Institute's mission.

  To facilitate the development of effective collaborations with partners across the community, the Institute will continue to proactively engage and bring together key personnel for small "blueprint" workshops on specific R&D topics. During these blueprint workshops, the partners will not only inform each other about the status and goals of various projects, but actively articulate and document a common vision for how the various activities fit together into a coherent R&D picture. The scope of each blueprint workshop should be sized in a pragmatic fashion to allow for convergence on the common vision, and key personnel involved should have the means of realigning efforts within the individual projects if necessary. The blueprint process is by design flexible and nimble to react to needs of the community. As a specific example, during the *Learning from the Pandemic: the Future of Meetings in HEP and Beyond* workshop [22] experiences with HEP virtual events during the COVID-19 pandemic were shared and ideas for best practices in future meetings were developed, including the hybrid format for event participation which is increasingly common in HEP.

  The ensemble of these blueprint workshops will be a process by which the Institute can establish its role within the wider HL-LHC R&D effort. The blueprint process is also a mechanism by which the Institute and its various partners can drive the evolution of the R&D topics over time.

- **Coordinated Ecosystem Workshops**: In contrast to the Blueprint Activity which runs topical workshops, IRIS-HEP (and its precursor S^2I^2 conceptualization process [4] which paved the way for the Institute) ran three "Coordinated Ecosystem Workshops", in 2017, 2019, and 2022 (the third workshop was delayed due to the COVID-19 pandemic) which focus on the entirety of the field's R&D. Each workshop consists of a broad overview of major activities across both DOE and NSF followed by breakouts to coordinate sub-areas. The goal of the workshop is to identify potential topics of collaboration (identifying commonalities that may have been overlooked due to differences in funding agencies or experiment), help the community develop a prioritization of projects based on its needs and science opportunities, to identify gaps in the current ecosystem, and to avoid starting unnecessary duplicate projects. The Institute will continue these series of workshops and consultant with the community on whether their frequency should be increased to annually and whether they should organize discussions around an expanded set of science drivers.

More generally, the Institute will continue to support activities which develop the capacity within the larger HEP and related communities to build and support larger **research software collaborations** whose products are relevant not only for LHC, but more broadly. Research software is a key intellectual product of our research, not just a critical tool. IRIS-HEP has inspired other such efforts and their ongoing success will be an impactful and important legacy of the Institute. This includes in particular support for activities of the HEP Software Foundation, but also building relevant collaborations with other more recently related funded national and international community research software projects that can build on our experience.

4.3 Institute Role in the Software Lifecycle

Figure 5 shows elements of the software life cycle as viewed by the NSF Office of Advanced Cyberinfrastructure (OAC), from *research* in core concepts and algorithms, through *development* of prototypes to deployment of software products and long term support as part of *sustained production*. The community vision for the Institute is that it will focus its resources on the late development stage (with some exploratory work in interlinked late-research / early-development software projects) and, in the years closer to the start of the HL-LHC, it will partner with the experiments, the U.S. LHC Operations Programs and others to transition software into sustained production. Compared to IRIS-HEP, the Institute would have more of these investments in the later stage of the lifecycle. The experiments already provide full integration, testing, and deployment in their internal lifecycle processes. The Institute will not duplicate these, but instead will collaborate with the experiments, the Operations programs, and the OSG Consortium on the efforts required for software integration activities and activities associated to initial deployments of new software products. This may also include the phasing out of older software elements, the transition of existing systems to new modes of working and the consolidation of existing redundant software elements.

The next phase of the Institute will have a finite lifetime of 5 years, ending immediately before the start of the HL-LHC; this is still much shorter than the planned lifetime of HL-LHC activities Thus, close coordination with the U.S. LHC Operations programs - which will last as long as the US participation in the HL-LHC - will be essential to ensure the longevity and sustainability of the Institute's projects. In its role as an intellectual hub for HEP software innovation, it will provide advice and guidance broadly on software development within the entire HEP ecosystem. This will be achieved through maintaining a critical mass of experts in scientific software development inside and outside of HEP and the cyberinfrastructure community who partner with the Institute.

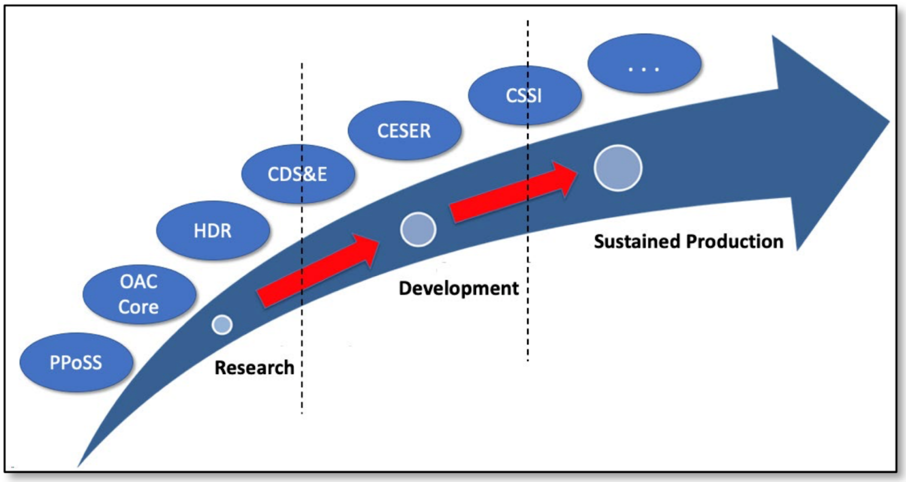

Figure 5: The Software Life Cycle as seen by NSF; the Institute will bridge projects from earlier research and development phases into sustained production. Figure reproduced from "Blueprint for a National Data and Software Cyberinfrastructure" by NSF OAC [23].

4.4 Institute Elements

The next phase of IRIS-HEP will have a number of internal functional elements, as shown in Figure 6.

Institute Management: To accomplish its mission, the institute will have a well-defined internal management structure, as well as external governance and advisory structures. Further information on this aspect is provided in Appendix B.

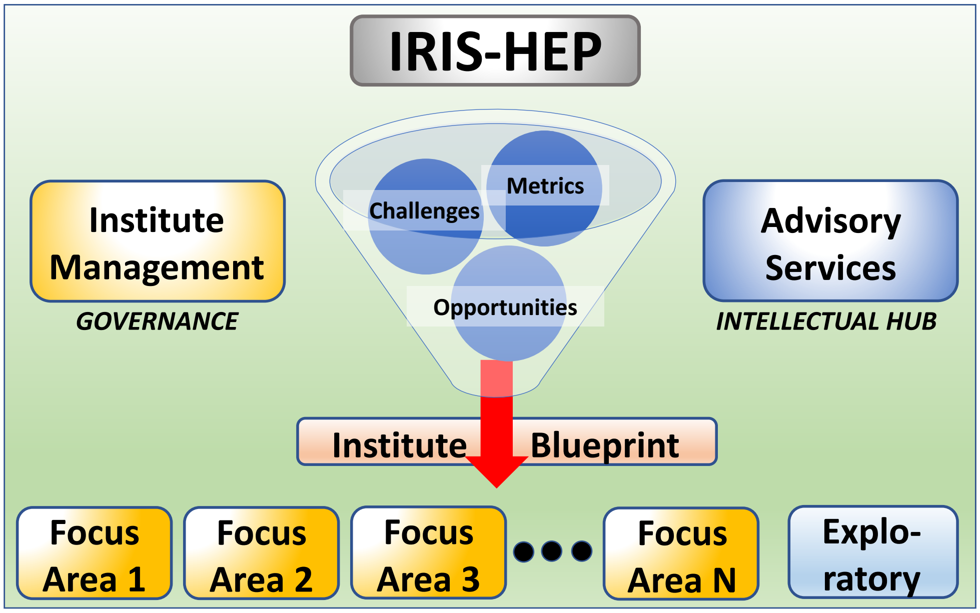

Figure 6: Components of the IRIS-HEP software institute. The focus areas envisioned for a follow-on Institute are given in Section 5.

Areas: The Institute will have 7 interconnected areas of activity, which will pursue the main goals of the Institute; these are described in Section 5. The final number of areas will be contingent on available funding (see Section 8). Each focus area will have its own specific plan of work and metrics for evaluation.

Blueprint & Sustainable Software Activity: The Institute's Blueprint Activity will maintain the software vision for the Institute and, 3-4 times per year, will bring together expertise to answer specific key questions within the scope of the Institute's activities or, as needed, within the wider scope of HEP software and computing. Blueprint activities will be an essential element to build a common vision with other HEP and HL-LHC R&D efforts, as described in Section 4.2. The blueprints will then inform the evolution of both the Institute activities and the overall community HL-LHC R&D objectives in the medium and long term.

Exploratory: Occasionally, the Institute may deploy modest resources for short term exploratory R&D projects of relevance to inform the planning and overall mission of the Institute.

Advisory Services: The Institute will play a role in the larger research software community (in HEP and beyond) by being available to provide technical and planning advice to other projects and by participating in reviews. The Institute will execute this functionality both with individuals directly employed by the Institute and by involving others through its network of partnerships.

Institute WBS Area	**Effort (FTE)**
Management/Project Office	1.9
Analysis Systems	10.4
DOMA	2.9
Innovative Algorithms	8.9
Sustainability & Training	1.4
Scalable System Laboratory	1.3
OSG-LHC	5.2
Total	**32.0**

Table 2: FTE distribution as of Year 5 of the current IRIS-HEP award/project, grouped by "Work Breakdown Schedule (WBS)" areas.

5 Strategic Areas of Activity for the Institute

As an Institute focused on the software and services required to ensure the scientific success of the HL-LHC, IRIS-HEP is part of a larger international research, development, and deployment community. It directly funds and leads some of the R&D efforts, supports related deployment efforts by the experiments, and it serves as an intellectual hub for more diverse efforts. In a potential second phase for IRIS-HEP from 2023-2028, the Institute's effort will be organized with the following focus areas:

1. **Analysis Systems**: Modernize and evolve tools and techniques for analysis of HL-LHC data sets. The Analysis Systems area will concentrate on *G3 (Analysis at scale)* topics of managing order-of-magnitude larger data sets, enabling more complex techniques including use of modern machine learning, and the adoption of data science tools toward *G4 (Sustainability)* goals. Deliverables will include the tools supporting a full pipeline for distributed columnar data analysis at scale that are interoperable with other elements of the HEP and broader data science ecosystems. Modern machine learning techniques and operations, including differentiable analysis pipelines, will be integrated, as well as full support for analysis preservation and reinterpretation.

2. **Reconstruction and Trigger Algorithms**: Develop and evolve pattern-recognition software able to exploit next-generation detector technologies, computing platforms, and programming techniques to accurately and efficiently identify charged particle trajectories. Efforts in this area are key to eliminating *G1 (resource)* gaps due to new, and more capable, experimental apparatus, larger data rates, and evolving computing hardware. Algorithms must be engineered to be adequately *G4 (sustainable)* over the course of HL-LHC operations. This area will deliver critical components of the tracking pipeline, prioritizing algorithmic interoperability, achieving high levels of parallelism, and implementing robust algorithms. Both traditional and novel approaches to tracking algorithms will be considered as tracking is a multifaceted problem and has optimization points that vary depending on the experimental apparatus design and computing technical design.

3. **Translational AI**: Exploit Machine Learning approaches to improve the physics reach of the HL-LHC. The Translational AI area will leverage fundamental research, such as the work done by the NSF AI Institutes, and focus on helping the HL-LHC experiments translate these capabilities into production. Activities include working to enable and use ML-based services, helping the field connect to available infrastructure, and working on enabling the "retraining" of in-use models for new data.

4. **Data Organization, Management, and Access (DOMA)**: Scale and modernize the bulk data transfer infrastructure including new authorization schemes, transfer protocols, and network integration; provide new data delivery services and techniques for use in analysis facilities. DOMA contributes to the *G2 (Scalability)* computing gap to close the 20x difference in the wide-area data rates expected between now and the start of the HL-LHC. DOMA innovates new authorization schemes for inter-site bulk data transfer coordinates international data challenges to mark progress toward the target data rates and integrate new technologies. For analysis, DOMA will develop services to deliver columnar data and to provide modern data management techniques from the database community to HL-LHC analysis environments.

5. **Facilities R&D**: Innovates new approaches to building facilities for the U.S. LHC and aligns the community with approaches in the larger NSF coordinated cyberinfrastructure. The area works with Kubernetes as a "substrate" to orchestrate portable services, provides testbed facilities to projects within the Institute, and investigates the use of multi-site Kubernetes clusters to provide agility to the operation of distributed services. Facilities R&D contributes to the *G4 (Sustainability)* goal by reducing the operational complexity and costs and to *G3 (Analysis at scale)* by applying agile techniques for future analysis facilities.

6. **Fabric of distributed high-throughput computing services (OSG)**: Operates a fabric of services specifically to meet the needs of the LHC and provides a stable route to their evolution for the HL-LHC. The OSG-LHC group ensures the needs of the LHC experiments while making contributions to the larger consortium, allowing the LHC to benefit from broader common services as well.

7. **Training, Workforce Development, and Outreach**: Executes and coordinates a broad range of events to help with the training, workforce development, and outreach needs of the HL-LHC community. The area in the Institute will ensure there is training available at multiple levels of need (undergraduate, graduate, postdoc, professional) and will run the IRIS-HEP Fellows program, a in-depth virtual mentoring program targeting senior undergraduates and junior graduate students. This is key to bridging the *G4 (Sustainability)* gap.

These areas of activity were chosen primarily based on the *impact* an investment could have on the HL-LHC Computing Gaps as outlined in Section 3.1 as well as continuous input from the community through workshops (Appendix A), the IRIS-HEP Steering Board and our numerous direct collaborators.

While the strategic areas are broad - touching areas from the instant an event is read out from the detector to the final publication of science results - they are joined in their efforts to close the computing gaps for HL-LHC as outlined in Section 3, and, after the first phase of IRIS-HEP, intertwined and inter-reliant. The software developed in DOMA for the production infrastructure is largely released to the LHC facilities through OSG-LHC. The Facilities R&D area provides extensive support for the testing and scaling of Analysis Systems components. An activity like the Coffea-Casa prototype analysis facility crosses OSG-LHC, DOMA, Analysis Systems, and Facility R&D. Another cross-cutting activity is the support of the LHCb experiment, which is at a different phase in its lifecycle compared to ATLAS and CMS. Accordingly, in Section 5.8, we aggregate together the LHCb activities that would be distributed throughout the areas of the institute. Even places that have little explicit connection such as reconstruction algorithms and OSG-LHC benefit from Institute structures like the project management and the intellectual hub which organizes Blueprint activities. The institute-based approach provides the long-term vision, structure, and alignment between distinct activities that is otherwise impossible as a collection of small projects.

5.1 Analysis Systems

Analysis Systems (AS) builds the tools, libraries, and pipelines that empower a physicist to transform an experiment's production data for physics results. These approaches can be, and are, used for LHC analysis, though the primary goal is to unlock the ability to perform at the scale and complexity of the HL-LHC era. While today's tools will still function in 2029, the scale alone would make HL-LHC cost prohibitive: some analyses today are already difficult to finish during a PhD student's tenure. Increasing the event count by 20x during the exploratory phase would effectively put analysis out of reach for many groups.

This presents the LHC community with a severe computing gap (*G3 (Analysis at scale)*), Section 3.3): the current approach to analysis will not scale to the HL-LHC dataset sizes and resource constraints. To address this issue, IRIS-HEP has worked to build an analysis ecosystem on the foundation of the vibrant and large open source Python data science community, which is used abundantly in industry, and has been a driving factor in modern approaches to data analysis in astrophysics and geoscience [24]. The ecosystem consists of individual sustainably developed analysis tools that aim to improve the analyst user experience, as seen in Figure 7. The focus on consistent APIs and common data exchange formats means this ecosystem is interoperable by design, allowing efficient and highly scalable workflows and data analysis pipelines — from data ingest to final statistical analysis — to be formed by integrating these tools. This development focus means the tools lend themselves to having cleaner interfaces, which is a key ingredient for analysis reuse and reinterpretation.

An end-to-end pipeline involves much more than just software tooling. Services are needed to deliver data and facilities are needed to have a "home" where users can run analyses at much larger scale than they do today. Efficient delivery and analysis execution requires close integration across the DOMA, Facilities R&D, and Analysis Systems teams. To facilitate such a collaboration, IRIS-HEP has put together the Analysis Grand Challenge (AGC); see Section 6.1. The AGC is a set of integrative, increasingly difficult exercises which prepares the combined teams for HL-LHC scale analysis. The ultimate goal of these exercises is not only to enable the largest university teams to do HL-LHC analyses but to empower smaller, under-resourced teams, broadening the participation in the scientific endeavour.

Specific Challenges and Opportunities

In the remaining R&D period between now and the HL-LHC, work on improving, optimizing, and integrating the Analysis System tools with each other and others in the broad HEP analysis ecosystem is crucial. There are also exciting new opportunities: integrating Machine Learning (ML) applications into the analysis pipelines in a natural way, improving our reinterpretation capabilities, and implementation of a fully differentiable analysis pipeline.

User experience for HL-LHC analyses: The AGC is an ideal testbed for tool integration and performance tests. The AGC is currently using a $t\bar{t}$ cross section measurement as an analysis demonstrator. The relatively straightforward analysis has given valuable feedback to the community showing, for example, work needs to be done to improve how data is handed between various stages of the analysis as well as improving the user experience for large distributed workflows. However, tool and integration development work needs to be done to properly handle systematic uncertainties and make the approach more realistic. To add more realistic challenges in the next phase, the AGC will adopt new flagship analyses for high-data-volume and high-complexity cases. Adding analyses that use even larger datasets, similar to the $t\bar{t}$ ℓ+jets mass measurement, and analyses that will use ML techniques, like the Higgs self-coupling measurement, will further exercise aspects of the integration.

Integration of Machine Learning (ML) into the Analysis Pipeline: Machine Learning techniques play an increasingly important role in analysis. By the HL-LHC almost every analysis

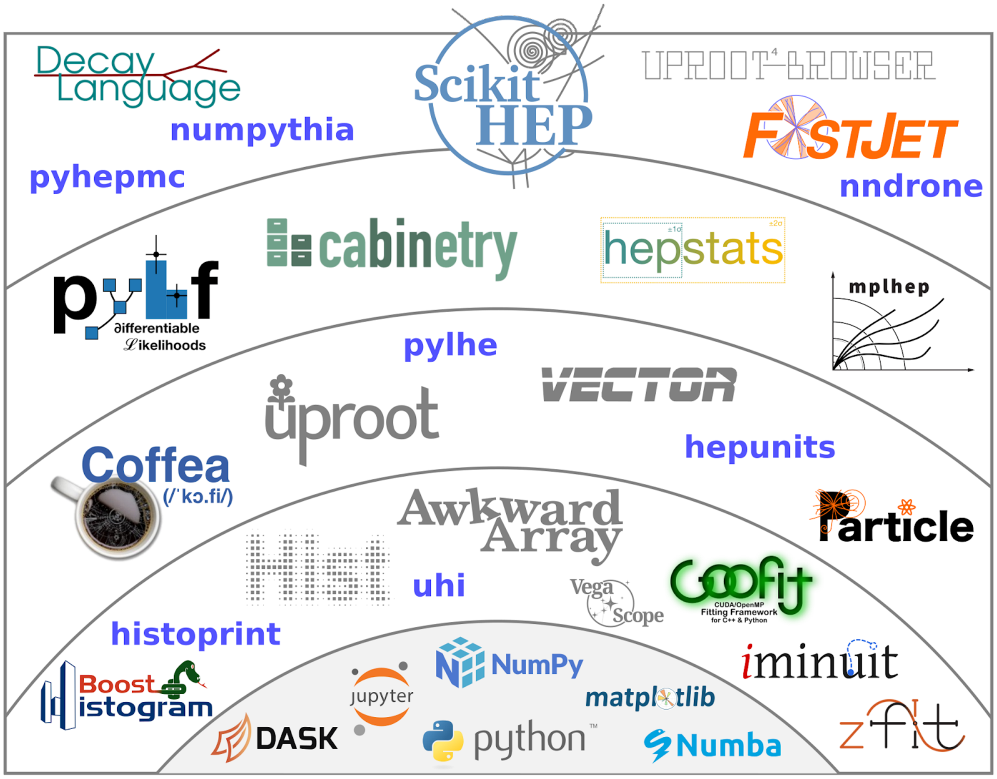

Figure 7: The components of the Python-based analysis ecosystem for HEP. The bottom ring consists of broadly popular libraries from the Python Data Science ecosystem. The rings surrounding the bottom contain tools that are more specifically designed for particle physics analysis and applications; while the bottom HEP layer is broadly used, each layer becomes more analysis- or experiment-specific. Many of the HEP-specific tools are part of the Analysis System pipeline and are either owned by or receive contributions from IRIS-HEP.

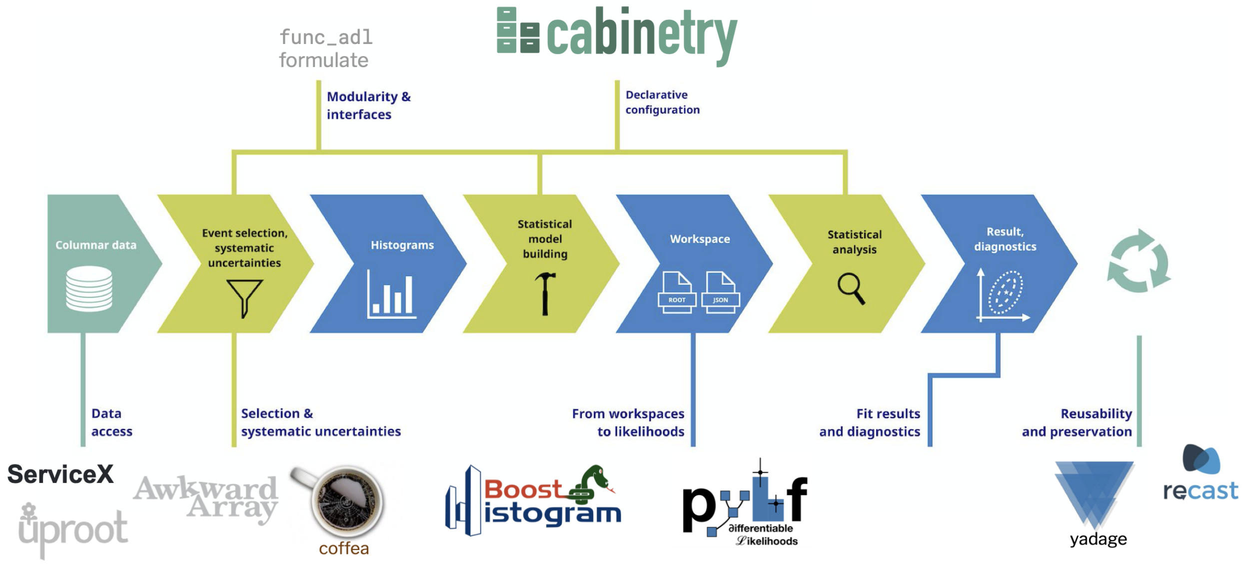

Figure 8: Representation of the Analysis Systems analysis pipeline. The projects shown represent the primary tools used that must integrate together to efficiently perform the analysis.

will depend on ML to improve physics sensitivity and reach. There are many stand-alone tools to aid with building, training, optimization, and deployment of ML models (e.g. MLFlow or KubeFlow), along with the more traditional approaches commonly used in the community. There are numerous impedance mismatches between the approaches resulting in analyzers solving the same tooling problems repeatedly. Given the centrality of ML in the ATLAS and CMS HL-LHC programs [25–27] and the institute's extensive work and expertise designing analysis workflows, folding in ML tools and services coherently into the overall ecosystem presents an opportunity for improving the user experience for analysts using ML.

Analysis Reinterpretation: Reinterpretation of physics analyses is a key technique to extend the physics reach of existing analyses. It allows the physicist to rule out newly proposed models using previously published analyses and extend the reach of analyses using new observations. Re-running a complex workflow requires all the steps to be portable to new environments and a workflow language specification to connect the steps. The REANA reproducible analysis platform [28], is used to orchestrate the workflows across distributed resources at scale. REANA fits well with a batch-oriented workflow and its unclear how it and other preservation services will need to adapt for newer services and tools. The challenge will be balancing innovation for new analyses while maintaining the important reinterpretation capabilities for the field.

Fully differentiable Analysis System pipeline: ML techniques have historically been applied in isolation in particle physics analyses. Neural networks are often trained as a final analysis discriminant to optimize for signal and background separation, though ML techniques hold even more potential for analysis. For example, systematic uncertainties are not included in the training which means that the network optimization may depend on variables for its separation power that are not well understood. Expanding network training to include information from other parts of the analysis — like information from the likelihood function used for sensitivity analysis and systematic variations of nuisance parameters — requires the analysis pipeline to be fully differentiable so that gradient calculations can be passed between stages. The neos project [29] has demonstrated the value of differentiable analysis systems by optimizing a simplified example analysis with respect to the expected sensitivity with a process that is aware of the modelling and treatment of systematic uncertainties [30,31]. The complete vision for Analysis Systems would have the full pipeline end-to-end differentiable, from analysis pre-selection cuts to the final sensitivity determination. Though an end-to-end differentiable analysis has never been accomplished, making it difficult to evaluate the full impact of the approach, including the systematic uncertainties in a current analysis has shown a preliminary improvement in sensitivity.

Current Approaches and Development Roadmap

Integrating HL-LHC analysis with the Data Science Ecosystem

Funding Scenarios [1]: Low (reduced scope), Medium, High
Description: The quality of the experience between a physicist and their analysis environment is important. Historically, physicists have been trained to write analysis code and then submit it to batch computing systems and wait for their results to be returned. In its first phase, IRIS-HEP began examining alternate approaches that arose from the data science world of task-based computing, notebook interactive computing environments, and expressive query-based languages as tools to tighten the analysis feedback loop and make data exploration more interactive. Analysis Systems built upon existing robust data science tools, primarily from the Python ecosystem, and created a HEP-orientated ecosystem of interoperable Pythonic data analysis tools, as seen in Figure 7. The tools of this ecosystem were then arranged into an analysis pipeline, as seen in Figure 8, based on their data analysis operations and functionality to enable a coherent flow of data between each stage of a physics analysis. The Uproot package [32] provides the data access to the ROOT [33] data files delivered by ServiceX [34] and the rest of DOMA, which are transformed into jagged Awkward Arrays [35] where they are manipulated for efficient array-based computations. The func_adl query language [36] allows for expressive event and kinematic selection criteria to be defined in analysis logic and processed in Uproot, then given to the Coffea columnar analysis framework [37] for additional processing, ultimately delivering histograms of the analysis selection in the form of boost-histogram [38] objects. These histogram objects are serialized and then ingested by cabinetry [39] to create statistical models of the physics processed in the analysis, which are then efficiently fit using cabinetry's robust selection of APIs for common analysis tasks, powered by pyhf's efficient statistical inference and optimization techniques [40,41], resulting in final summary statistics for the analysis. Analysis Systems synthesizes efficient data analysis pipelines from the integration and interactions of these HEP data science tools, which coordinate closely with each other to ensure robust interoperability and efficient computations while also allowing for expressive operations and exploration as standalone tools. Their design allows them to also extend the reach and functionality of the Analysis Systems pipeline through interactions with additional tools in the data science world (e.g. Awkward and Dask, pyhf and JAX).

As discussed more in Section 5.6, with the trend of increasing heterogeneity in the hardware market, Analysis Facilities are expected to support more ARM-based resources as well as GPUs in addition to more traditional computing architectures by the start of the HL-LHC [25–27]. The broader data science and machine learning worlds have been following these market trends and expanding tool support from traditional x86 architectures to include multiple ARM-based platforms. Similarly, industry machine learning frameworks are beginning to expand support across multiple commercial GPU architectures. By integrating with and expanding on the Python data science ecosystem Analysis Systems is well poised to exploit these trends. Many of the Analysis Systems tools already provide support for ARM-based platforms and the statistical tools already support hardware acceleration on commercially available GPUs. It is anticipated that as ML will

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[1] Throughout this section, we annotate each activity with associated funding scenarios (low scenario - \$4M/year, medium / baseline - \$5M/year, high - \$6M/year). These indicate the scenarios where IRIS-HEP would work on the activity. This particular activity would be supported in all expected scenarios; in some cases, such as the this one, in lower funding scenarios the scope and scale would be greatly reduced.

become a more common component of multiple stages of analysis and more analysis tools will be able to leverage hardware acceleration the demand for GPU resources will grow (discussed further in Section 5.4). Investment now in additional GPU resources at Analysis Facilities will allow for ML workflows and services to become mainstream parts of analysis workflows and reach production levels of integration before the start of the HL-LHC.

Current and Potential Future Activities:

- *New data formats*: A new data format, RNTuple, is being developed for the field as part of the ROOT toolkit. Basic reading of this data has been implemented in Uproot, but the access methods are not user-friendly and RNTuple writing has not been completed. As the RNTuple format is still evolving, Uproot's implementation will need to evolve with it. Additionally, as the Apache Parquet and Apache Arrow data formats are being considered for fast columnar data access in ATLAS and CMS [25–27], ServiceX, Awkward, and Coffea's existing compatibility with them allows for Analysis Systems pipelines to immediately explore analyses with these new formats.
- *Supporting heterogeneous compute resources*: As heterogenous compute resources become more abundant at Analysis Facilities and across the field supporting these platforms becomes more critical. Analysis Systems tools already largely support multiple ARM-based platforms and are expanding coverage for operations resources.
- *Supporting columnar data analysis*: The Analysis Systems analysis pipeline is built on a columnar analysis approach and exploits Awkward and Coffea's design choices. Supporting columnar data access and analysis infrastructure are planned HL-LHC milestones for ATLAS and CMS. As work towards these milestones advances, AS tools will need to adapt to support interoperability with the experiment solutions (e.g. implementations in ROOT's RNTuple, ATLAS's PHYSLITE, and CMS's NanoAOD). [25–27]
- *Filling missing serialization gaps*: Interoperability between components in an ecosystem is critical for user experience. While most analyses could be converted to pure Python, there are key object types that cannot be cleanly serialized / deserialized from within Python (e.g. ROOT's 'member-wise serialization' mode, RooFit models, boost-histogram objects). By closing these gaps, the next phase of IRIS-HEP can better serve HL-LHC user communities that use these techniques.
- *Maturing tools to production*: While most of the Analysis Systems tools have become mature projects and staples of the Scikit-HEP community [42] with stable APIs, large user bases, and contributions from outside of the development teams, there remain edge cases in terms of features as well as user experience and knowledge that need to be addressed to reach a production state. Covering the full range of Analysis Grand Challenge exercises, in addition to supporting LHC analyses already using Analysis Systems tools, provides a roadmap for reaching a feature-complete production state as well as opportunities for strengthening synergies with Scikit-HEP and coordination with facilities and US operations. Forming community investment and knowledge for the Analysis Systems tooling ecosystem is also required to reach a production state where the HEP community can contribute to the long term maintenance of projects beyond the scope of IRIS-HEP operations (*G4 (Sustainability)*), Section 3.4). Analysis Systems is addressing this in multiple ways:
  - Training the community: By participating in the community training and workforce development events coordinated by IRIS-HEP (described in Section 5.7) Analysis Systems is able to educate the HEP community on the tools and workflows being produced, while also receiving direct user feedback on the user experience. Analysis Systems is also closely involved with the activities of the HSF working groups, with multiple members serving as co-conveners for the HSF Python in HEP (PyHEP) working group. PyHEP

holds an annual online workshop covering the state of Python in the field with in-depth tutorials for widely used tools. Analysis Systems tools have become recurring highlights of the workshop tutorials, which have hundreds of daily active participants and historically over a thousand registered participants, allowing for updates on latest techniques, workflows, and developments to be shard with the HEP user and contributor community.

  - Engaging the broader scientific open source community: Some Analysis Systems projects, like Awkward, provide functionality that solve uses cases typical enough in scientific computing that the user base has extended beyond HEP to other scientific fields and industry. This has lead to a collaboration with engineers at the data science company Anaconda to create dask-awkward [43] which allows Awkward arrays to be used natively in Dask computational workflows. To further adoption in the broader data science community and foster closer interactions with the open source tools the Analysis Systems ecosystem builds upon, multiple tools have applied to become "affiliated projects" with NumFOCUS [44] — a non-profit community organizing body for promoting open practices in research, data, and scientific computing which includes member projects like NumPy, SciPy, Jupyter, and Numba. pyhf is the first IRIS-HEP project to be accepted as an affiliated project of NumFOCUS in 2022, with other projects expected to be accepted in 2023. Collaborations with industry and the open source data science community allow for Analysis Systems tools to develop diverse contributor communities and maintenance support systems.

> Providing high levels of interoperability between components of the Analysis Systems ecosystem with each other and with external data analysis libraries is one of the most high-impact activities of the Analysis Systems team.

Statistical Tools for HL-LHC
Funding Scenarios: Low (reduced scope), Medium, High
Description: The statistical inference demands for analyses at the HL-LHC will require tools that are able to fit large and complex statistical models efficiently. This implies tools must become easier to use — physicists should be able to build complex statistical models quickly using expressive APIs — and be able to better leverage available hardware accelerators to avoid the statistical step from becoming a bottleneck. In the first phase of IRIS-HEP, the pyhf Python library was adopted for its ability to leverage hardware acceleration and automatic differentiation for faster fits. Similarly, the cabinetry Python library was developed to build on top of pyhf and enhance the model building experience and provide high level APIs for statistical procedures common to HEP. The next phase of statistical tooling will focus on *adding functionality* that will be necessary for HL-LHC and for a fully differentiable Analysis Systems pipeline as well as *optimizing the performance* of the libraries for statistical inference on GPUs.
Current and Potential Future Activities:

- *Fully differentiable analysis pipeline*: pyhf uses machine learning frameworks to exploit automatic differentiation of the constructed likelihood function to speed up statistical inference. The computational graph that is created for this currently remains internal to the calculation and extending this to provide passing of gradient information from pyhf to other libraries requires additional work. The neos project builds on pyhf to provide an example implementation of a subset of the necessary changes to be able to differentiate through pyhf-based calculations, and will serve as an external comparison for pyhf's development, as well as a future external user for validation.

- *Hardware acceleration optimization*: The first phase of IRIS-HEP prioritized the user experience of fitting statistical models on GPUs rather than the performance optimization. A focus on improving the performance across its GPU-enabled computational backends is expected to deliver 2x or more speedups. This optimization work would provide opportunities to strengthen the relationship between the IRIS-HEP team and NVIDIA software engineers working on their RAPIDS AI product.
- *Adoption of unifying statistical model standards*: The High Energy Physics Statistics Serialization Standard (HS3) [45] — which will allow for unification of model specification across the HEP statistical landscape — has recently been proposed and outlined by maintainers of tools in the HEP statistical modeling ecosystem, including the pyhf developers, with a planned publication of the new specification the end of 2023. Having pyhf and cabinetry support the HS3 standard would allow for increased interoperability (*G4 (Sustainability)*), Section 3.4) and remove the need for model serialization conversion between pyhf and other statistical libraries like RooFit and Bayesian Analysis Toolkit (BAT) [46].
- *Efficient orchestration of template histogram production*: cabinetry provides convenient high level APIs for building and steer template fits, however at the moment the template histogram production steps are sequential and not optimized. This can be a bottleneck when approaching analyses with a large number of systematic uncertainties as this requires repeated sequential reads and compute operations for each systematic variation applied. The larger analyses of the HL-LHC will require cabinetry to have optimized read and decision operations based on variations in addition to efficient parallelization of histogram production.

The performance, flexibility, and interoperability of the Analysis Systems statistical tools presents opportunities for significant impacts on HL-LHC analysis.

Analysis Preservation and Reinterpretation
Funding Scenarios: Medium (reduced scope), High
Description: The physics value of ensuring that LHC and HL-LHC analyses are preserved in a robust and complete state such that they are usable for reinterpretation of new physics signatures is significant. In addition to reducing the analysis team time for investigation of new physics models, it reduces the total compute needed compared to an analysis being created for the first time. Additional work will be required to find ways to map the analysis preservation and reinterpretation technology that exists for the current LHC analyses to the Analysis Systems workflows that have been designed to run on Coffea-Casa infrastructure, or, alternatively, to map the entirety of an AGC-like analysis into a computational node in a larger analysis reinterpretation workflow (i.e., implemented with REANA).
Current and Potential Future Activities:

- *Coordinating development of analysis preservation and reinterpretation technology*: IRIS-HEP Analysis Systems team members are developers of the RECAST software [47], used for ATLAS's complete analysis preservation approach, and coordinate with the REANA development team to ensure compatibility of RECAST and REANA releases. This coordination work and development work will be extended to also include support for and integration of Analysis Systems workflows with these existing technologies.
- *Development of Coffea-Casa compatible reinterpretation workflows*: To ensure that the AGC analyses preserved with modern HEP technologies do not limit the analysis computation, exploration of the implementation paradigms is required. One approach is to embed the entirety of the analysis as a node in a larger reinterpretation workflow (i.e. in REANA),

but would present additional deployment restrictions. An alternative approach is to develop approaches that allow for the current preservation and reinterpretation technologies workflow graphs to be executed within Coffea-Casa infrastructure for tighter integration. It is unclear which is the correct implementation paradigm and requires exploration of options and then engineering of an appropriate solution.

Enabling Differentiable Analysis for HL-LHC
Funding Scenarios: Medium (reduced scope), High
Description: A goal of Analysis Systems is to make performing more advanced analyses easier and faster through considered design of the tools and well executed implementation. Often selection optimization with respect to a specific variable is performed in analyses at the LHC, but it is performed by variations in incremental discrete steps. Being able to differentiate through the selection step allows for exact optimization of the variable, and similarly if the entire analysis toolchain is able to be differentiated through the entire analysis can be end-to-end optimized by optimizing the final discriminant with respect to the model parameters. This is a large scale project that will require new development and design effort for all core Analysis Systems projects (Awkward, Uproot, func_adl, Coffea, histogram libraries, pyhf, and cabinetry) and will be an excellent integration exercise for Analysis Systems.
Current and Potential Future Activities:

- *Supporting automatic differentiation in AS tools*: To achieve a fully differentiable Analysis Systems pipeline requires that all components are able to handle differentiable operations as well as the propagation of gradient information. There are ongoing efforts to add automatic differentiation support for Awkward and expose pyhf's internal automatic differentiation to other operations, though implementing support for the remaining tools and then efficiently integrating all the tools to support end-to-end optimization requires substantial development work.

ML Integrated with the Analysis Pipeline
Funding Scenarios: Medium (reduced scope), High
Description: As analysis scale and complexity grows at the HL-LHC the use of machine learning in all aspects of analysis will grow as well. It is critical to be able to support ML workflows at any stage of the Analysis Systems pipeline and to have clear examples of how ML workflows and applications can be integrated into the existing pipeline.
Current and Potential Future Activities:

- *Integration of ML operations into AGC analyses*: There are ongoing efforts to expand the AGC benchmark analyses to also include ML components. The first stages of this involve taking ML models that are used widely by the LHC experiments and integrating their deployment as an additional stage of the Analysis Systems pipeline. In addition to this initial step, adding support for ML models to be trained efficiently on GPUs on Coffea-Casa infrastructure and then used directly in the Analysis Systems pipeline will also be required.
- *Provide MLOps infrastructure*: The process of being able to robustly retrain machine learning models, test and evaluate them, and then deploy in a versioned manner into a production analysis environment (broadly known in machine learning research as “MLOps“) requires substantial orchestration and maintenance. As the Analysis Systems ecosystem and pipelines are designed to be extensible to allow analysts to quickly iterate on analyses without constraining them, providing MLOps for Analysis Systems would allow for faster integration of user ML models into analyses. Providing MLOps infrastructure requires development of expertise and software infrastructure in MLOps system development and deployment, but presents large added value for turnaround times on physics analyses that rely heavily on ML approaches.

MLOps implementation will be a point of close collaboration with Facilities R&D to ensure efficient use of GPUs and other compute resources without interruption or added burden.

- *Support high level ML workflows*: In addition to MLOps infrastructure users will need high level workflows that allow them to iterate through the ML lifecycle — from experimentation to deployment to the Analysis Systems pipeline — in a reproducible manner. Open source MLOps orchestration tools like MLFlow and KubeFlow have been developed by industry to make it easier for researchers to manage the complexity of the end-to-end process of building and deploying ML models. Leveraging these industry standards to create reproducible workflows quickly will provide an improved user experience for physicists using complex ML models for analysis.

Handling complex data with Awkward Array

Funding Scenarios: Low (reduced scope), Medium, High
Description: One hallmark of HEP data is its complexity; it is fundamentally deeply nested, uses variable-sized arrays, records, mixed types, and missing data from records. This has made HEP data difficult to use with standard data science tools like NumPy, which often assumes fixed-sized, rectilinear data. Awkward Array fills this gap, providing a NumPy-like interface to this so-called "jagged" data. Awkward has reached a state of maturity and has an ecosystem of tools that are being built around it, including with non-HEP-specific focus like the collaboration with Anaconda. It is foundational in the infrastructure built by IRIS-HEP and the Analysis Systems pipeline is built on top.
Current and Potential Future Activities:

- *Supporting automatic differentiation*: A fully differentiable pipeline requires Awkward-array and to be able to perform operations that propagate gradients through calculations. This will require additional substantial development work.
- *Speeding up calculations*: Awkward provides users with natural Python interface to HEP data; now the interface is established, increasing the overall speed is critical. While its NumPy-like interfaces are *much* faster than native Python, it has not achieved the same speed as native C++ code. A C++ JIT backend — where operations can be combined and lowered directly to machine code — would eliminate many of these issues.
- *ROOT integration*: Outside Python, the defacto toolkit for data analysis is ROOT. The AS team aims for smooth interoperability between ROOT and the rest of the ecosystem. For example, ROOT's RDataFrame approach to analysis needs to be extensively tested and potentially expanded when processing Awkward Arrays.

> Complexity of data and analyses at the HL-LHC will grow. Planned improvements to Awkward Array will provide the data handling and manipulation capabilities necessary to approach these challenges.

Impact and Success Criteria

In the first stage of IRIS-HEP, Analysis Systems has provided leadership in the end-user facing HEP software community, with members of Analysis Systems holding convenerships in the HEP Software Foundation Python in HEP working group and administrator roles in the Scikit-HEP community project, and provided a nucleation site for software discussions — generating many of the IRIS-HEP Blueprint Activity meetings and driving development discussions and best practices in the IRIS-HEP Slack. The largest impact Analysis Systems has had is providing mature, interoperable analysis software that physicists at the LHC experiments have been able to adopt already into their workflows and analyses. Most notably, the Coffea project used actively for analysis in CMS is not an IRIS-HEP project, yet has adopted many components of the Analysis Systems ecosystem — including Awkward, Uproot, and hist — as core dependencies to better integrate into the analysis design philosophy of Analysis Systems, which also affects analyses in CMS. Additionally, as of December 2022, the pyhf library has been used by ATLAS to publish 24 full statistical models of published ATLAS results, and become a core dependency of analysis frameworks used in the ATLAS SUSY group for ATLAS Run II results. While the adoption of collections of individual components of the Analysis Systems is a step forward, the realization of the full benefit of Analysis Systems comes from the integrated use of the ecosystem as a whole. Investment in Analysis Systems as part of an NSF-funded software institute will bring more LHC analyses into strong positions for adoption of Analysis Systems pipelines before the HL-LHC begins and allow for the full impact of the analysis ecosystem designed and built in the first phase of IRIS-HEP on the landscape of modern physics analyses. Having Analysis Systems as a focus area brings momentum and ecosystem continuity, with existing teams of IRIS-HEP developers ready to build on the success of the analysis ecosystem and community.

The high-impact outcomes for analysis activities in Analysis Systems will be tightly coupled with the success and participation in the AGC. The AGC will provide multiple opportunities for demonstration of the planned Analysis Systems milestones, covered in detail in Section 6.1, including implementation of the high-complexity di-Higgs search AGC analysis that will exploit the added machine learning components of the Analysis Systems pipeline and the improvements in statistical tools. The capstone of these demonstrations will be the 2026 AGC demonstration of a fully differentiable analysis which will leverage advances across the Analysis Systems ecosystem. These demonstration efforts will compound in value as they additionally serve as roadmaps to full adoption of Analysis Systems pipelines for the LHC experiments.

Success Criteria – Milestones & Deliverables:

The milestones and deliverables outlined below focus on the first three years of an Institute. These high-level items would be expanded and later years filled in as part of the execution of any project.

D4.1. All core components of the Analysis Systems pipeline fully support distributed analysis. **May 2024**.

D4.2. Demonstration of running a full analysis, that is suitable for addition to the AGC, that uses machine learning. **July 2024**.

D4.3. Demonstration of running a full analysis, that is suitable for addition to the AGC, that is able to use statistical models defined in the unified HS3 serialization format (planned for release at the end of 2023). **December 2024**.

D4.4. Demonstration of the Analysis Systems pipeline being used as part of a reinterpretation workflow (e.g., a node within a larger graph executed the REANA analysis platform). **December 2024**.

D4.5. All core components of the Analysis Systems pipeline support integration of differentiable operations and passing of gradients. **July 2025**.

D4.6. Demonstration of reinterpretation of an AGC analysis through use of a reinterpretation platform. **December 2025**.

D4.7. Demonstration of an analysis, suitable for addition to the AGC, that has been optimized end-to-end through use of automatic differentiation of the Analysis Systems pipeline. **December 2026**.

Success Criteria – Metrics:

Metrics are a useful tool to provide management with quantitative insight about progress toward overarching goals. High-level metrics we expect to be applicable for the Analysis Systems area are below:

M4.1. The number of users and analysis groups that use Analysis Systems tools and/or pipelines in early stages of analysis. Collecting feedback from these early adopters allows to understand better user experience related issues. The goal is to add at least two analyses per year.

M4.2. The number of Analysis Systems tools that support integration with automatic differentiation. The goal is half of all relevant projects by December 2023 and all relevant projects by end of December 2024.

M4.3. The number of analyses that use machine learning that are able to perform aspects of model training or run model inference as part of the Analysis Systems pipeline. The goal is one by the end of July 2024, and one from each target LHC experiment by the end of July 2025.

M4.4. The number of publications, conference notes, or public notes from each of the target LHC experiments that cite the use of the Analysis Systems tools and analysis pipeline. The goal is at least one by the end of December 2024, and at least one from each target LHC experiment by the end of December 2025.

M4.5. The number of Analysis Systems tools that have at least one regular contributor or maintainer from the broader scientific developer community. The goal is at least one for each project that is undergoing active feature development — projects that are at a mature stage of their life cycle and only providing bug fix releases are not expected to have additional non-IRIS-HEP maintainers.

5.2 Reconstruction and Trigger Algorithms

Algorithms unpack raw detector data and transform it into data structures that can then be used to identify interesting events: either in real-time by the software *trigger* system, or later during *reconstruction* prior to analysis. These algorithms are run in three distinct contexts by the LHC experiments. First, in the software trigger system, where a keep or reject decision must be made for around one million events per second during standard data taking conditions in HL-LHC. This process is challenging as only around 1% of these events (or 0.01% of the total collision rate of LHC) can be retained. Second, these algorithms are run 'offline' (outside of the detector environment at CERN) to reconstruct data providing data in experiment-specific data formats to analysts. Third, these algorithms are run to reconstruct Monte Carlo simulations to provide the same data formats to analysts. Together these use cases drive the computational processing needs of HL-LHC experiments. While already true during Run 3, the resource needs of these algorithms increases more quickly than other aspects for several reasons. First the event rates, both into the software trigger system and out of it (and into the offline) are expected to grow substantially. More importantly, the event complexity - driven by the number of simultaneous overlapping 'pileup' events that occur at each *pp* interaction will increase by a factor of three to four; the reconstruction computational cost scales approximately quadratically with the pile up. Finally, to achieve the needed science reach for HL-LHC, more advanced – and at the same time more complex – detectors are required.

All three effects drive up the computational processing resources needed for the planned HL-LHC physics program.

Amongst the online trigger and offline reconstruction algorithms, the most resource intensive ones are the *tracking* algorithms: algorithms that together identify where charged particles have traversed the inner part of the detector and their kinematic properties. This is no surprise as the number of electronic channels to be digitized from our detectors for each bunch crossing is dominated by those of the inner tracking detectors. Despite being the focus of continuous research during Run 1 and Run 2 of LHC, the compute needs of traditional approaches continue to increase rapidly with increased event complexity and require significant innovation. This re-engineering – in some areas, a complete rethinking of the approach – is central to ensuring the HL-LHC physics program and a critical factor affecting the scale of processing power needed both the online and offline environments.

Specific Challenges and Opportunities

For pattern recognition algorithms, the period between now and the start of HL-LHC is a time for research consolidation and algorithm integration into the experiment's trigger and event reconstruction pipelines. Work involves making algorithms more robust and more easily maintained as well as the process of algorithm validation.

Incorporating abstraction libraries Code written for the HL-LHC will need to last a decade or more – three or more generations of a typical supercomputing environment. It becomes costly to write against low-level vendor libraries; the more flexible our algorithms can become, the more sustainable they will be as hardware (particularly, accelerators) radically changes. To function efficiently throughout the HL-LHC program we need to identify the best approaches for the largest cross-section of algorithms. We plan to adopt the strategies decided on by the field, for example the results from HEP-CCE, in cases where a consensus has been reached. One possible development path forward is the use of abstraction libraries, such as Alpaka, Kokkos, etc, that can effectively compile kernels for the set of hardware architectures that they support.

Algorithm interoperability While developments of new tracking algorithms typically happen outside of the context of a full tracking pipeline, their ability to interoperate with this full pipeline is critical. One example is data structures that are well suited for data exchange between algorithms. Another is having the flexibility to minimize data movement across a heterogeneous infrastructure. Interoperability aspects are critical as algorithms mature and are adopted by experiments into their full tracking pipeline.

Algorithm design and optimization Algorithms must be designed and evolved to exploit parallelism, have optimized data structures, and use compute and memory efficiently. Tracking algorithms must expose as many parallelization opportunities as possible to the underlying environment. Exposing parallelism is mandatory to make use of accelerators but are also important for CPU-based approaches where instruction-level parallelism is required to use all the available silicon effectively. Given stagnant improvements in memory latencies and bandwidth compared to the computational power, the use of optimized data structures greatly affects algorithmic performance. This includes both data exchange between tracking algorithms and from tracking algorithms to the subsequent steps in the workload. Considerations here include efficiency for data access in highly parallel environments, optimized CPU-to-GPU data movement, and to ensure vectorized calculations can be performed. As algorithm developments mature and turn to integration and optimization, they should undergo a tuning process to reduce compute and memory needs. This is typically best done when data exchange and algorithm interoperability aspects can be properly included in the analysis.

Machine Learning approaches to tracking ML has the promise of delivering novel, innovative algorithms. However, a key milestone is understanding how these algorithms can provide a better or more sustainable approach to improved speed or physics performance for particular aspects of the tracking pipeline. Graph Neural Networks (GNNs) are the current best candidate approach, however the broader ML research community should be followed to identify new opportunities now that our community has a better understanding of the strengths and weaknesses of ML approaches applied to tracking problems.

Integration and validation Integration of a new algorithm or approach into an experiment is extraordinarily challenging; impressive performance improvements count for nothing if the whole dataset must be reprocessed due to a bug in the code. Trigger algorithms are even more conservative: an improperly rejected event is lost forever! The acceptance and adoption of low-level algorithms can be a long and time-consuming process. Experiments have therefore set up a detailed validation process to evaluate and eventually adopt new algorithms. Given their complexity, these processes require close and intensive collaboration with developers realize the benefits and in this regard institutes like IRIS-HEP with its significant resources, long time scale and broad vision can play a unique role.

Current Approaches and Development Roadmap

The primary focus for the next phase of the Institute will be maturing research directions and begin consolidation of the work for each experiment's tracking program for HL-LHC. Multiple algorithmic approaches will most likely make up the tracking for each experiment, experiments may take a different approach online than offline, and experiments may take different choices from each other. These are all natural choices, as tracking is a multifaceted problem (seed finding, track finding, track fitting) and has optimization points that vary depending on the experimental apparatus design and computing technical design (e.g., fast and approximate online vs best-possible precision offline).

ACTS development and integration

Funding Scenarios: Low (reduced scope), Medium, High

Description: A Common Tracking Software (ACTS) project is an international, open-source project developing an experiment-independent set of track reconstruction tools. The main philosophy is to provide high-level track reconstruction modules that can be used for any tracking detector. The description of the tracking detector's geometry is optimized for efficient navigation and quick extrapolation of tracks. Converters for several common geometry description languages exist. Having a highly performant, yet largely customizable implementation of track reconstruction algorithms was a primary objective for the design of this toolset. Additionally, the applicability to real-life HEP experiments plays major role in the development process. Apart from algorithmic code, this project also provides an event data model for the description of track parameters and measurements. Key features of the project include: tracking geometry description which can be constructed from standard community geometry libraries a simple and efficient event data model, performant and highly flexible algorithms for track propagation and fitting, basic seed finding algorithms.

Current and Potential Future Activities:

- *Full track reconstruction chain*: Within IRIS-HEP, the primary focus has been on the development of core track reconstruction algorithms within ACTS and its application to the ATLAS experiment. ACTS is foreseen to be the replacement for the current ATLAS tracking algorithms for the HL-LHC because it will provide speed advantages by exploiting modern C++ and built-in multithreading. At present, a number of algorithms have been developed and the integration of ACTS into Athena (the ATLAS physics framework) is ongoing. The major milestone will be to run a full track reconstruction chain on the ATLAS ITk geometry within athena. Once this has been achieved a detailed assessment of the physics and computational performance can be made and the algorithms can be tuned.

- *Machine Learning and hardware acceleration*: ACTS has R&D lines which are pursued in parallel to the main project. The traccc project is developing a demonstrator of an end-to-end track reconstruction algorithm that runs on GPUs. Algorithms, such as the seed finding, which have already been ported to GPU, have demonstrated promising speed improvements, however the full end-to-end track reconstruction chain is needed to prove if GPUs are an appropriate choice for HL-LHC.
- *Tracking in the event filter trigger*: ATLAS is currently exploring different options for tracking at the event filter level. One possible option would be using ACTS as part of a fully software-based event filter trigger. IRIS-HEP has already dedicated a small amount of person-power for exploratory R&D and this is an exciting avenue for the next phase. Both the CPU and GPU versions of the code will be explored and the performance compared between the two. The adoption of ACTS for the trigger would decreases long-term maintenance costs for the ATLAS experiment as a single code base would be used for online and offline track reconstruction.

mkFit development and integration

Funding Scenarios: Low (reduced scope), Medium, High
Description: MkFit is a re-engineering of traditional Kalman Filter tracking to leverage the capabilities of modern CPU architectures. Most of the research to date has been on the most time-consuming tracking components, trajectory finding. MkFit has advanced sufficiently to become the baseline tracking for CMS in Run 3 and is used to find more than 90% of CMS tracks. For these tracks, the trajectory finding is now significantly faster than the track fitting algorithms, which illustrates potential benefits gained by re-engineering conventional algorithms to match modern compute architectures.
Current and Potential Future Activities:

- *Kalman parameter fit*: Evaluating methods to apply the mkFit approach to the final Kalman parameter fit. This includes evaluation in the context of CMS data structures appropriate for vectorization-aware CPU algorithms or accelerators.
- *Consolidating and achieving algorithm speed up*: The mkFit software was deployed in production as part of CMS's Run 3 software; we expect to apply lessons learned from initial 2022 deployment and apply improvements for HL-LHC geometry.
- *Improving interoperability within CMS tracking chain*: While mkFit was developed as a standalone project, it is ultimately meant to operate efficiently within the CMSSW framework. For example, in the next phase we will design efficient mechanisms to take track seeds from modernized pixel tracking (the "Patatrack" algorithm [48] as input.

Line Segment Tracking development and integration

Funding Scenarios: Low (reduced scope), Medium, High
Description: Line Segment tracking (LST) is designed to take advantage of the CMS-specific tracker detector layout which includes doublet layers. This geometry allows track segments to be initially found within each set of doublet layers, a process which is highly parallelizable. These doublets can then be linked together to create track seeds and eventually full track candidates. Initial implementations of this algorithm are inherently parallel, implemented already on NVIDIA's CUDA GPU programming language, and should be easily portable to other accelerator platforms.
Current and Potential Future Activities:

- *Mature algorithm*: The LST approach shows potential to meet both speed and correctness requirements necessary for CMS in the HL-LHC era. However, an open research question is precisely how much speedup remains achievable; more work is needed to increase the "realism" of the implementation (removing simplifications and scaffolding that were used to first demonstrate the original concept) and achieve the desired impact.

- *Adopt hardware abstraction layer*: The current R&D version of the LST algorithms were written using CUDA; it cannot be run on non-NVIDIA resources such as those available on DOE's (AMD-based) Frontier, currently the fastest supercomputer in the world. A hardware abstraction library will be required for an algorithm to survive through the HL-LHC era.
- *Increasing parallelism*: The current LST algorithms are memory-hungry compared to what's available on modern GPUs (and what might be affordable during the HL-LHC era). The amount of work assigned per GPU device - and hence the total parallelism and speedup of the algorithm - is limited by the available memory, leaving GPU cores idle. An initial goal of the next phase is to reduce the memory footprint to fully leverage the available silicon.

Machine Learning approaches to tracking
Funding Scenarios: High
Description: Unlike traditional tracking approaches, a GNN pipeline scales linearly, not quadratically, with data density – making it an interesting option for the HL-LHC environment. Various research efforts have established pipelines for researching GNN architectures and training approaches applied to different tracking algorithms. While these have not caught up to the technical (speed) or physics (accuracy) performance relative to the highly-tuned existing algorithms, they are rapidly advancing and potential remains to help close the raw resource gap for HL-LHC.
Current and Potential Future Activities:

- *More Compact GNNs*: Evaluating novel GNN techniques and have focused partially on the inner detector (pixel-based) tracking. Small and thus quick to evaluate GNN architectures are promising but need further research to reach adequate physics performance. One important use case is the online system, where computational speed is more important than precision.

Defining tracking pipelines for ATLAS and CMS
Funding Scenarios: Medium, High
Description: Individual algorithms are insufficient; they must be combined into full tracking pipelines. The performance challenges for this process are in the data exchange at algorithm boundaries as well as balancing overall physics performance with computational costs.
Current and Potential Future Activities:

- Experiments are in the process of defining tracking pipelines over the next five or so years. For example, a likely vision for CMS tracking in HL-LHC is one that begins with pixel seeds created by Patatrack, then unpacking / clustering of the outer tracker information and matching outer tracker hits using LST. The combination of these two could be done on an accelerator which avoids the costly moving data between GPU memory and main memory. After these steps, a more traditional Kalman filter approach via mkFit would then be used to complete the track finding and do the final track fitting. This setup would be appropriate for both online and offline environments and they could meet the differing goals of the two applications through different configurations. Piecing together such a pipeline requires active involvement of algorithm developers to properly configure and optimize it.

Impact and Success Criteria

Investment into the research of techniques for pattern recognition algorithms – specifically charged-particle tracking algorithms – will enable a tracking approach that meets the goals of the HL-LHC scientific program; perform within the resource budget used for Run 3 tracking; and be flexible enough to exploit evolving computing hardware through the HL-LHC era. Primary success metrics are related to achieving superior *technical performance* and delivering superior *science performance* relative to state-of-the-art algorithms and other R&D approaches:

- **Performance**: Both online and offline, the critical metric is event throughput per unit (compute) cost. Given current performance estimates, a factor of two reduction in the full tracking pipeline would translate into a 25% reduction in compute for CMS at the HL-LHC. Large factors have already been demonstrated in individual tracking algorithms through ongoing research. Now developments must realize these gains in practice. In the next phase of IRIS-HEP, our research aims to **achieve factors of two to three in speedup of critical tracking algorithms** in both the offline and trigger environments.
- **Correctness**: Physics performance – computing the "correct" result for the underlying inputs – is critical. The HL-LHC program sets a minimum threshold of algorithm's physics performance to have the desired scientific reach. This is particularly critical as tracking underlies many other reconstruction components, meaning that deficiencies will propagate throughout the physics data formats for analysis. Given the excellent physics performance of current algorithms, the primary goal for this metric is to maintain current levels while focusing on improving potential gaps. Gaps foreseen include tracking efficiency in particularly dense environments (eg, in high-p_t jets), for highly displaced tracks (eg, from long-lived particles), and to further reduce the level of fake tracks (tracks "found" by the algorithm that were not part of the actual physics).

Tracking code written but not adopted by the experiment has minimal impact. Unlike the analysis environment, where a variety of approaches are taken by different groups, each HL-LHC experiment can only afford to run one set of the most resource-intensive tracking algorithms online and offline. The next five years will include a long process of evaluation and decision making to define the basis for HL-LHC tracking within each experiment. This process must be tracked in order to facilitate adoption of promising research directions and to cut short those that will not be adopted; **the structure and long-term view of an institute is critical for the desired impact**.

Research in algorithms for event reconstruction and trigger applications build upon numerous previous and still on-going NSF investments and serve as an excellent training ground for early-career HEP researchers. For example, three postdocs in this area who were associated to IRIS-HEP have since taken faculty positions: Philip Chang is now faculty at the University of Florida (worked on LST tracking at UCSD); Xiaocong Ai is a professor at Zhengzhou University (worked on ACTS at UC, Berkeley) and Dylan Rankin is a professor at Pennsylvania University (worked on hadron calorimetry reconstruction algorithms on accelerators at MIT).

HL-LHC Computing Gap Impact: Research in Reconstruction and Trigger Algorithms impacts gaps *G1 (raw resource usage)* and *G4 (Sustainability)*. As a major consumer of resources - estimated to be a majority consumer in the case of CMS - investment in this area has the largest impact in closing the resource gap. To be sustainable, implementations must be both flexible and adaptable across hardware platforms and generations. High-energy physics depends on being able to make effective use of both specialized high-performance (online) and commodity (offline) hardware as well as high-performance computing. Today this means having codes engineered well enough to be adapted to new hardware architectures either through an interoperability layer or by other means. As the LHC community has no control over the hardware market, and only indirect control over the hardware architectures at the distributed resources, tracking algorithms must design in mechanisms to support hardware architectures most prevalent during the HL-LHC era. HEP detector designs will continue to evolve beyond the initial HL-LHC phase. In the energy-frontier, there is R&D for both future colliders and so-called phase-3 LHC upgrades; the software should be sufficiently adaptable to be used for these or other future experiments. While achieving the ultimate performance from tracking algorithms in a specific detector geometry typically requires detailed tuning, algorithms which seek applicability beyond a single experiments must demonstrate how easily they can be used by another and whether there is any trade off in performance.

Success Criteria - Milestones & Deliverables
D2.1 ATLAS demonstrators (2024,Q2). The ATLAS experiment is currently defining a list of demonstrator projects. Selected demonstrators need to be released by Q2 2024 after which time they will be evaluated by the experiment for physics performance, technical performance and overall readiness.

D2.2 CDR/TDR documents of experiments (2024). Both experiments have a timeline to prepare documents describing their software and computing model for HL-LHC and to submit documents to support the LHCC review of the WLCG. Performance and readiness of potential tracking algorithms is an important component of these documents.

D2.3 Downselect and validation by experiments (2026 or later). Transitions from research to evaluation and validation by experiments must be complete for final adoption by experiments. Timelines will be established closer to the start of HL-LHC operations.

Success Criteria - Metrics:
M2.1. Number of deployed tracking algorithm components that meet or exceed the performance requirements of the HL-LHC science program.

M2.2. Number of deployed tracking algorithm components that achieve factors of two or more reduction in resource needs for HL-LHC in either the offline and trigger environments.

M2.3. Number of deployed tracking algorithm components that are able to run efficiency with abstraction libraries as adopted by experimental frameworks.

5.3 Translational AI

Cutting-edge research in artificial intelligence and machine learning – "AI" for short – directly benefits the physics program of the HL-LHC. In many ways, AI is transforming the way field does physics. A dedicated effort in Translational AI will increase adoption of promising new techniques and reduce the time and effort needed to deploy these solutions in the experiments. This would significantly impact all aspects of HL-LHC physics, including trigger, reconstruction, simulation, and analysis.

HEP has a long history of using AI and has been very active in embracing and contributing to modern AI research. The field has developed experts in AI and is beginning to see wider adoption of the techniques by non-experts.

New AI techniques are able to work with the complex, low-level data, which generally enhances performance or sensitivity compared to traditional approaches. Similarly, new AI techniques targeting simulation, multivaraite unfolding, and anomaly detection are providing qualitatively new capabilities that can change the HL-LHC physics program in more fundamental ways.

Exploratory AI R&D is often done outside of experiments. This work occurs in the context of other NSF projects like IAIFI [49] and A3D3 [50], or in small research teams, or is explicitly funded as part of experimentalist's base physics research grants. There are a number of barriers to the adoption of this research in the experiments. For example, the papers written by AI researchers are often not easily translated into the HEP context without the aid of expertise in both fields - making them accessible only to the ML experts within the field. Even if the papers are accessible, the implementation of the new techniques require further development to be adapted to the experiment's context. Finally, the integration of ML techniques into an experiment's workflow is often accomplished with bespoke solutions, and often different groups within one experiment will approach this differently.

> The faster the community can absorb new AI research and translate it into use by experiments, the more impact it will have on the physics program.

Ad-hoc collaborations and communication between AI research groups and experiments have formed around collaborations between AI and particle physics researchers. These links have grown a small, but active, group of AI experts in particle physics. The communication does run in both directions: as particle physics provides opportunities for use-inspired research in AI, these collaborations do influence AI research resulting in work that is well-matched to the field's problems. This healthy communication must be maintained and strengthened as the field must find ways to bring advanced techniques to a broader audience. Graph Neural Networks (GNNs) are an illustrative example. This type of AI model is particularly well suited to our problem space. A multidisciplinary team including physicists and AI researchers at Deep Mind have prepared a review article and position piece outlining this development [51]. GNNs are now used for bottom-quark identification [52], replacing an RNN-based solution, and are being explored for tracking, jet reconstruction, and tagging. However, there are many advances remaining before GNNs could be a solution for tracking (see Section 5.2).

Coordination is needed to guide the evolution from this period of rapid R&D, prototyping, and bespoke solutions for deployment to a more mature and established set of practices for ML in various contexts (e.g. trigger, reconstruction, simulation, analysis). US funding agencies have invested resources in making foundational progress in AI. This new strategic area will improve the research deployment pipeline, help to further normalize the use of ML, and provide a set of best practices that can be used by all researchers, not just experts.

Specific Challenges and Opportunities

The challenges and opportunities that will help transform how ML is used at the HL-LHC can be split into three broad categories.

Bringing research from the AI Community to the HL-LHC: Most AI research happens outside the experiments. For example, a team of Computer Science or Statistics researchers will develop a new technique. Another common pattern is that of a small team, including some people from the HL-LHC community and some people from CS, will use greatly simplified detector data to publish a paper directly addressing problems in the field. The new techniques are not easily incorporated into the experiment. Currently, bespoke solutions are employed for development, training, and deployment. Worse, the target environments - trigger, reconstruction, and analysis - all require different solutions for inference. There is an opportunity to work with the AI research community and the particle physics community to build tools that span the domains and make the inclusion of new AI techniques more straightforward.

The NSF and DOE fund a large amount of foundational AI research. Two NSF institutes, IAIFI and A3D3, are good examples of this work. IRIS-HEP's broad reach via its intellectual hub role and work on Analysis Facilities and training infrastructure provide opportunities for bringing this research into the field.

Improving HL-LHC's interaction with the AI Research Community: Our problem space is interesting to AI researchers. Delivering realistic data to the researchers in a way that a non-domain expert can understand is not easy, however. This is further complicated by some experiments not wanting to release their simulation data openly. Finally, it is desirable to use experiment-agnostic data when collaborating with AI researchers. A toolchain exists to generate experiment-agnostic data [53], but it does not fully represent the complexity of an HL-LHC detector, and it writes data in a field-specific format (ROOT). Improvements to these tools and data formats will make collaboration simpler. With this work and a better understanding of the challenge and benchmarking tool set, the community can participate in public challenges more effectively and collaborate more easily with non-HEP AI research teams.

Sustainable AI at the HL-LHC: The AI landscape is evolving rapidly. New techniques replace old ones. People move from one task to another or leave an experiment entirely. As AI is used more and more in reconstruction and the trigger, it becomes important to have a process in place to maintain it. The data streaming from the detector will evolve over the course of the HL-LHC (expected to run more than a decade) - due to changes in the position of the detector components or due to radiation damage, for example. The retraining of such a mission-critical ML algorithm cannot be dependent on a (former) student's laptop configuration. The field needs to develop infrastructure and best practices around the long-term sustainability of ML algorithms in reconstruction and the trigger.

Current Approaches and Development Roadmap

Translational AI will be a new area for IRIS-HEP, and there is already a tremendous amount of work on AI in the field. IRIS-HEP has at least two places it can offer a unique contribution that play to its already existing strengths: helping to bridge the foundational AI research community and HL-LHC physicists, and helping to build sustainable AI within the experiments. The work to accomplish this first relies on building consensus in the field and then helping to execute on that consensus. It is a mix of blueprint meetings and concrete development projects. It would be a new area for the next phase of IRIS-HEP, having appeared in the initial S^2I^2 strategic plan but being largely de-scoped due to available resources. Some of the tasks are important for the long-term sustainability of the experiments and will have to be solved by the field; IRIS-HEP can make important cross-experiment contributions and help set the direction for the community. The current work and roadmap is much more exploratory than in the other areas of this strategic plan as this is a new area for IRIS-HEP and a covers a lot of ground the field has not yet given careful thought to.

Training and Community

Building Community Consensus

Funding Scenarios: Medium
Description: Holding **Blueprint meetings** (as part of the Intellectual Hub activity in Section 4.2) will help build community consensus and guide the exploratory activities in this area. These meetings will work to improve the understanding between experiments and groups in the experiments and also explore best practices from outside the field of particle physics and improve collaboration with the AI research community. The activities listed below are all meetings planned to help bootstrap the activities in this new area.
Current and Potential Future Activities:

- *Streamlining ML Data Delivery*: Different cyberinfrastructure is used to process data during prototyping, training, and deployment. Frequently, the methods and code to extract the input data to build training/prototyping datasets are different from the way the same task is performed for a deployed solution. A common set of tools to address this will reduce deployment time and may allow uniform access to national or international resources for complex training. This work may also allow caching of training datasets reducing the DOMA burden.
- *Deploying Trained Models in different environments*: There are experiment hardware and software experts for the trigger, reconstruction, and analysis. Each is a radically different environment in which we wish to run ML algorithms. The way ML is prototyped and deployed in each is quite different, resulting in drastically different infrastructure. This meeting will understand the different environments and explore how to make the training environment as common as possible.
- *Using the AI Benchmarking and Challenge infrastructure in HEP*: With the overall goal of using more common tools in training, deployment, benchmarking, and challenges, this blueprint meeting will bring together the various communities to understand the current state-of-the-art and how it could evolve to help quickly move new ideas and solutions between communities. There is a lot of community expertise already existing. Challenges and benchmarking efforts are initiated, organized, and reported in workshops like ML4Jets, ML4PS, NeurIPS, Hammer & Nails, MODE, Aspen, IPAM, Dagstuhl, and MIAPbP. A recent DOE award, “A Fair Universe: Unbiased Data Benchmark Ecosystem for Physics”, is explicitly addressing the benchmark side of this story.
- *Disseminating Advanced ML Techniques within the field*: An advanced library of ML techniques - translations of ML papers - is hard to build. For most physicists reading an ML paper is difficult due to the different problem domains and vocabulary (sometimes even for the same concept!). Nor is it possible to have one or two people translate all papers into some sort of common example format as the approach won’t scale. This meeting will pull together people from similar institutes, such as the eScience Institute at the University of Washington (which actively deals with a similar problem), and experts within the field of particle physics to discuss scalable ways of pushing advanced AI techniques into the experiments.
- *Foundational Models*: Many areas of AI are adopting a pattern referred to as *foundational*

models, where a large, multi-purpose model is used as a common backbone for many tasks. While the foundation model may be expensive to train over large amounts of data, those costs are amortized over relatively inexpensive fine tuning or task-specific modules. Thus far, HEP has not adopted this pattern, but it offers potential advantages. However, it is also not clear that this pattern holds well for HEP use cases. A blueprint to explore this pattern would be valuable.

- *Prompt-based assistants based on language models*: Recently released models such as GitHub Copilot and ChatGPT, allow one to quickly translate instructions formulated as plain English text prompts into code or other actions. This blueprint meeting would gather experts on such models and experts from HEP and HEP/ML to develop a program of research that can be followed in the next years (in or outside of IRIS-HEP) to use the power of these new models.

Training and Dissemination

Funding Scenarios: High
Description: Getting advanced AI techniques into the hands of physicists requires a training program addressing multiple levels - especially when this must be scaled out to reach the full field of HL-LHC physicists. Many users of AI at the HL-LHC are still learning the basics - so their needs must be addressed in a way that they can later then use the more advanced techniques.
Current and Potential Future Activities:

- *Basic Machine Learning Skills*: The HEP Software Foundation and IRIS-HEP and many others collaborate on building a library of training resources for basic software skills using the Software Carpentry's model. The library already contains two ML-related trainings - one for basic PyTorch training and one using GPU's to accelerate training; advanced training materials will be added to cover LHC-specific topics instead of generic basic topics.
- *Advanced Techniques*: A library of example uses of advanced ML techniques will be built. This library will provide physicists who have absorbed the more basic training the ability to apply the techniques with best practices being integrated from the blueprint meetings.

Making Fundamental AI Research Sustanibly Work for the HL-LHC Experiments

Sustainable AI at the HL-LHC

Funding Scenarios: High
Description: Currently, AI solutions deployed in the experiments are rapidly replaced by new and improved solutions that are developed through a relatively ad-hoc process. As the AI solutions stabilize, systems will be needed to streamline the retraining or fine-tuning of these AI models in response to changing running conditions. This is akin to the routine recalibration and data reprocessing that the experiments manage, but brings in different computing challenges (access to GPUs, multiple passes over batches of training events, etc.) as the algorithmic patterns encountered in training are different than those found with recalibration. This also adds new requirements to the metadata that tracks run conditions and software versioning. There is an opportunity to design systems that can leverage computing resources that are well suited for AI, and reduce inefficiencies in the data transfer and redundancies that will be encountered without a more streamlined solution.
Current and Potential Future Activities:

- *Retraining Challenge*: Working with reconstruction authors within an experiment to use community tools to automate the retraining of a reconstruction component. Once implemented, track its use and updates required to keep it working as run conditions and the detector evolve.

Benchmarks and AI Challenges

Funding Scenarios: High

Description: Coordination is needed to guide the evolution from this period of rapid R&D, prototyping, and bespoke solutions for deployment to a more mature or established set of practices for ML in various contexts (trigger, reconstruction, simulation, analysis). There is an opportunity to establish the cyberinfrastructure components (both human and technical) that can serve as a bridge between the vibrant AI R&D activities taking place outside of the context of the individual experiments and the experiment-specific software and computing frameworks.
Current and Potential Future Activities:

- *Community Challenge and Benchmark Infrastructure Efforts*: Use the roadmap from the blueprint meeting "Using the AI Benchmarking and Challenge infrastructure in HEP" to form a program of work to better integrate challenge and benchmark tools in to the HL-LHC's ML infrastructure.
- *Using Common Infrastructure in the Experiments*: Close the gap between the backend infrastructure used for benchmarks and challenges and what is used in the experiments. The experiments have multiple environments that would require separate studies (trigger, reconstruction, analysis). Especially important will be supporting prototyping efforts as new techniques are explored inside the experiments.

Hardware Accelerators

Funding Scenarios: High
Description: R&D on AI with accelerators (e.g. FPGAs) and in highly constrained computing environments (e.g. trigger) requires both specialized hardware and specialized expertise. This poses a high barrier to entry and hinders participation from a more distributed and diverse group of teams. There is an opportunity to facilitate research and lower the barrier to participation by investing in a centralized resource with dedicated expertise and hardware to support distributed research on AI in these highly constrained computing environments.
Current and Potential Future Activities:

- *Making ML on FPGA's Accessible*: Work with the A3D3 institute [50] to best understand how to move their R&D work into a place where others in the experiment can make use of it. In particular, the software pipeline and testbeds that can be hosted at a community resource (e.g. an Analysis Facility). The goal of this work is to make the barrier of entry to developing ML trigger solutions lower.

Improving AI Research on HEP Data

Expanding connections between AI and HEP Communities

Funding Scenarios: High
Description: Data from HL-LHC detectors is ideal for many types of AI research. The problems that need to be solved (e.g. jet tagging, track reconstruction, signal identification) require learning complex processes, physics concepts, and even geometric relationships. Further, the problems solved can have large impacts on the physics ability of the HL-LHC and resource requirements. The common tools in the field to generate data suitable for ML are more tuned for internal use.
Current and Potential Future Activities:

- *Simulating a Generic HL-LHC Detector*: Tools like DELPHES implement a simplified simulation of an LHC detector. This tool set needs to be updated to reflect some of the complexities of an HL-LHC detector: adding more modern tracking architectures and an active calorimeter much like CMS's next-generation forward calorimeter. This work would also include building a more automated pipeline for producing datasets that could be used in challenges.

- *Data Formats For Research*: The data formats used by the HL-LHC community are mostly ROOT based, which is not easy for AI researchers and others outside the field to use. Tools like NumPy and Pandas DataFrames or Arrow Tables are more commonly used. This task will work on building these common formats as first-class citizens.
- *AI Challenges*: As the work above comes together this will enable the field to build and run AI challenges. Running a successful challenge is far from simple, however. Working with others within the field that have run challenges, a set of best practices will be built by example.

Impact and Success Criteria

Success Criteria – Milestones & Deliverables:

The milestones and deliverables outlined below focus on the first three years of an Institute. These high-level items would be expanded and later years filled in as part of the execution of any project.

D4.1. Each Blueprint meeting will have one of its products a report. A milestone will be associated with the circulation of the report to the community. The expected dates will be tied to the schedule (about 4 months after the occurrence of the blueprint meeting). **Various**

D4.2. Retraining Challenge completed: a ML algorithm, used in the reconstruction or trigger, has its retraining automated. **December 2025**.

D4.3. Launching an FPGA testbed (like SSL). **December 2026**.

D4.4. Run a Challenge with entrants from the AI Research Community. **December 2027**

D4.5. Access to a FPGA for ML training is possible on a Analysis Facility. **December 2027**

D4.6. A training is run locally and non-locally from the training and testing infrastructure. Normalizing training means that researchers can take advantage of GPU's for training around the world, or on the infrastructure hosting the training service, and have the same user experience.

Success Criteria – Metrics:

Metrics are a useful tool to provide management with quantitative insight into progress toward overarching goals. High-level metrics we expect to be applicable to the Translational AI area are below:

M3.1. The number of foundational trainings added to the HSF training library to help physicists incorporate ML into their workflows.

M3.2. The number of advanced ML techniques added to a library as exemplars for the field.

M3.3. Number of AI / ML models or use cases that are integrated into experimental infrastructure using the processes developed by the institute.

M3.4. Number of times the FGPA service at an Analysis Facilities are being used per quarter.

5.4 Data Organization, Management and Access (DOMA)

Given the centrality of ‘data’ to all things the HL-LHC will do, it is not surprising the investment area of data organization, management, and access is a key part of all four HL-LHC Computing Gaps. The immense volume of data is the easiest to conceptualize – starting with the predicted trigger rate, days of data taking per year, and event size, the HL-LHC experiments can make leading-order estimates of the raw, processed, and simulated data sets necessary for the desired scientific scope. Feed these numbers into the current resource requirement modeling and already the disk requirements needed outpace the fixed-budget scenario. The problems compound, however, once one takes into account this data must be moved about the shared national cyberinfrastructure, analyzed at much higher data rates than today at facilities, and done using common infrastructure to reduce sustainability costs.

Together, these challenges in the DOMA area illustrate the fact that HL-LHC science is not achievable by simply purchasing more servers, disks, and network switches - but otherwise leaving the approaches untouched. A robust R&D program is needed across both the production infrastructure and analysis facilities subareas of DOMA building upon the successes in the last 5 years. For bulk data movement, the entire LHC production infrastructure has migrated from the niche GridFTP protocol to the industry-standard HTTP, demonstrating the capability to both deliver from R&D to production and also execute system-wide changes. The community has planned and executed the first biennial data challenge, DC21, as part of the Data Grand Challenge (Section 6.2, showing the ability to coordinate on the global scale and provide integrative milestones for technology projects. Finally, during IRIS-HEP, the Coffea-Casa analysis facility platform was developed; Coffea-Casa provides a “first look” location for new analysis system services to intersect with users. The areas where the DOMA team has been active during IRIS-HEP are shown in Figure 9.

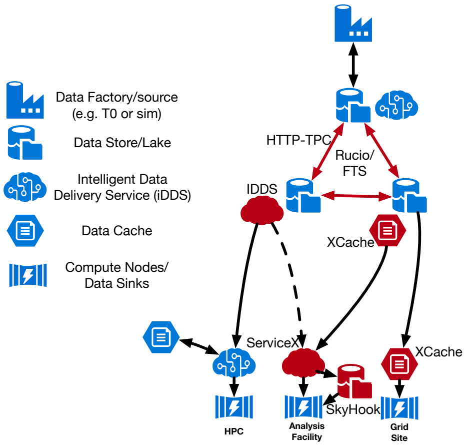

Figure 9: Schematic showing the DOMA-related components in the production infrastructure. The components that DOMA started or contributed to in IRIS-HEP are colored in red. The dashed arrow from IDDS to ServiceX is one of the planned projects for the next phase.

Specific Challenges and Opportunities

In the remaining R&D period between now and the HL-LHC, we see opportunities in the DOMA area continuing work in preparing the coordinated cyberinfrastructure or HL-LHC data volumes, transitioning to newer technologies used by industry and elsewhere in scientific computing infrastructures, and delivering data to analysis facilities.

Scaling up data volumes to HL-LHC: There is a need for innovation, development, and integration in nearly every service in the bulk data transfer infrastructure used by the LHC community to prepare it for the HL-LHC data volumes. Opportunities include benchmarking the existing software on available R&D testbeds such as the National Research Platform (NRP) [54], utilizing next-generation networks such as FABRIC [55], and leveraging engineered network paths as in the ESNet SENSE project [56]. The community has the opportunity to utilize these testbeds as a proving ground for techniques between the proposed biennial global data challenges (Section 6.2) and as part of any regional / US-specific exercises.

Technology transitions for bulk data movement: Several of the technologies historically used for the bulk data movement stack are at end-of-life, causing difficulty in the sustainability of the infrastructure. For example, the WLCG-wide tape archival protocol, Storage Resource Management (SRM), is based on a custom transport layer (not Transport Layer Security, TLS, which is ubiquitous across the Internet) and uses a remote procedure call protocol, SOAP, which is long out of favor. This has created a new opportunity to reconsider parts of the ecosystem - for example, the community has already replaced the use of the niche GridFTP protocol with the industry-standard HTTP - resulting in potential leaps in sustainability through leveraging industry standards. During the next 5 years, we see the following potential transitions necessary for the community:

- Moving the authorization scheme from identity-mapping based (mapping a credential to a local identity) to capability based (a credential is tied to a specific action). Capability-based schemes provide for more fine-grained authorization - only the actions intended for a job must be sent along with it. This transition requires coordinated changes across the software stack and integration in the ecosystem.
- Migrating bulk data movement to IPv6. IPv4 is considered a legacy protocol by the IETF meaning future innovations in the networking layer will be exclusively done for IPv6; the transition to IPv6 for all bulk traffic should be completed. For example, packet extensions that enable monitoring of network flows on ESNet are only defined for IPv6.

Delivering data to analysis facilities: The hallmark of HL-LHC analysis will be the size of the dataset (event count and volume), the need to deliver initial results at lower latency, and the use of a broader range of "data science" and machine learning tools from outside physics. The data volume and complex environment is expected to cause users to move from laptop-scale machines to analysis facilities that specialize in high-data-rate I/O, ML-support services (such as inference services), user interfaces (such as pseudo-interactive task-based computing or notebooks), and advanced data management services. These facilities, either from new approaches as in Section 5.5 or built on top of existing, batch-oriented analysis facilities, will need advanced data delivery and management services.

For example, an important trend in HEP analysis is the movement to Python tools and columnar analysis. In addition to giving analyzers experience with popular data science tooling, columnar analysis has the potential to unlock vectorization and performance benefits by defining operations on columns as opposed to individual events. To successfully leverage these analysis techniques, services are needed to filter, transform, and deliver columns to workloads running at analysis facilities.

HEP analysis has historically been a strongly filesystem-based activity: a user will take a dataset – often just a set of files in a directory – and apply simple transforms and filtering, resulting in a reduced set of output files in a new dataset. Users often make only simple changes, such as adding a few derived values to the event, meaning each of these derived datasets have a high level of overlap. Further, if a column was missing or incorrect in the original derivation, the user has to repeat the process from scratch. The system is wasteful of both disk space and – more importantly – physicist time. There are modern data management systems that provide the ability to do common database techniques such as virtual views and joins without needing to convert the ecosystem to a RDBMS; there is opportunity to both tap into a rich vein of industry investment (helping with the *G4 (Sustainability)* gap) in addition to making physicists more productive. As the management evolves, data delivery will similarly need to change to effectively schedule and pull the data from the wider distributed cyberinfrastructure into the facility and transform the data into the desired format for data management. This will require both services in the analysis facility and at the network layer (leveraging the NRP and SENSE work) to ensure proper prioritization and effective caching.

Integration point: Finally, the institute structure itself provides a unique opportunity. The DOMA ecosystem for the LHC and HL-LHC is large, complex, and slow-moving, making it difficult for independent smaller-scale research projects (such as those in the NSF CSSI Elements program) to deliver their work to production. The Institute's DOMA strategic area would be large enough to serve as an intellectual hub, connecting between innovative ideas coming into the NSF ecosystem, R&D testbeds at the national scale, and the production cyberinfrastructure for the HL-LHC.

Current Approaches and Development Roadmap

The DOMA area can be partitioned into investments into the production infrastructure, focused primarily on the HL-LHC Computing Gaps for sustainability (G4), scalability (G2), and raw resource requirements (G1), and the analysis systems investments, focused on sustainability (G4) and analysis at scale (G2). Below we outline existing approaches in each area.

Production Infrastructure Projects

Scaling the CI to HL-LHC data rates

Funding Scenarios: Medium (reduced scope), High
Description: From the beginning of Run 3 to the first full year of HL-LHC, the expected data volume moved per year by the LHC experiments will rise by 20 fold. To prepare for these data rates, the community has defined a set of biennial data challenges as described in Section 6.2. The data challenges are meant as capstones & milestones; the majority of the effort is in the preparation in the years leading up to the challenge. This project would work on the engineering and integration of community-wide research projects to demonstrate the readiness of the cyberinfrastructure for the HL-LHC scale.
Current and Potential Future Activities:

- *Demonstrating scaling of reference platforms*: The various software reference platforms (for IRIS-HEP, this is XRootD on top of a POSIX filesystem) used for bulk data transfer must be shown to scale well before trying load tests on production systems. NSF has funded a number of experimental storage (such as NRP, providing filesystems) and network (such as FABRIC, a 1Tbps platform between San Diego and New York) resources. By leveraging external R&D testbeds, the community is able to attempt tests at HL-LHC scales without needing to "buy ahead" at production facilities.
- *Leveraging engineered network paths*: By segmenting HL-LHC bulk data traffic onto specially-engineered network paths, the network connectivity providers (for US LHC, this is ESNet) have the ability to isolate user specified data flows, enhancing their accountability and at the same time allowing for prioritization, segmentation, and specialized quality-of-service techniques. ESNet's SENSE project [56] provides a mechanism for engineering the paths end-to-end; however, this functionality needs to be integrated into the LHC's data management software (Rucio) and shown to work across multiple sites.
- *Organizing US regional exercises*: The WLCG-wide data challenges provide a biennial global synchronization point for facilities and technologies. These require significant effort and coordination making it difficult to incorporate less mature technologies or regional concerns. We foresee a need to have US-specific regional exercises focused on technologies the US LHC is investing in (such as the Rucio / SENSE integration) and challenges such as integration with US HPC sites. An institute-scale DOMA strategic area, cross-cutting the HL-LHC experiments, would be uniquely situated to coordinate such exercises.

Scaling the cyberinfrastructure to close the 20x gap between today's and HL-LHC's expected transfer rates is one of the most high-impact activities of the DOMA team.

Authorization technology overhaul for the distributed infrastructure
Funding Scenarios: Medium, High
Description: Capability-based authorization provides a powerful new paradigm for asserting authorizations on a distributed infrastructure. Each experiment now has a token issuer service that asserts a specific action the bearer (hence the term "bearer token") can perform in the experiment's distributed resources; IRIS-HEP has worked to ensure the storage systems used by the LHC community interpret these assertions in an interoperable manner.

However, significant work remains to ensure all the software used by the community has been adopted to acquire, manage, and utilize these new credentials. These technologies remain a headline feature planned for the next data challenge to allow sufficient time for a complete transition by the start of the HL-LHC.
Current and Potential Future Activities:

- *Coordinating evolution of token usage & profiles*: While the intellectual approach to capability-based tokens was done in 2017 by the SciTokens project, significant coordination effort was required to expand the idea to cover all LHC use cases and to gain traction in the community. Common interpretations of authorization schemes is a strict requirement for establishing trust when moving data between sites; the DOMA strategic area has the opportunity to continue working with the WLCG authorization working group as the profiles evolve and are updated with technologies.

  Now the foundational work is done on the capability language, the community needs to better define the token acquisition and exchange workflows, for example, designing how they move from data management system (Rucio) to file transfer system (FTS) to storage endpoint.
- *Engineering a reference implementation*: The IRIS-HEP DOMA area provided a reference implementation for token-based authorization embedded in the XRootD server software. This is used by several LHC facilities and provides an endpoint for storage and middleware developers to use for testing their own independent implementations.
- *Provide leadership and support*: New technologies always pose a challenge for system administrators, providing expertise and a direction helps to ease the burden and make changes better welcomed by the community.

Organized delivery of data to running production workflows
Funding Scenarios: High
Description: In the first four years of IRIS-HEP, the DOMA area invested in the Intelligent Data Delivery Service (IDDS) which provided the ability to do data-centric workflows within the PanDA workflow management system. IDDS was used to help implement "disk carousels" (minimizing the use of disk buffers by the ATLAS experiment) and manage large-scale hyperparameter optimization runs; in impacts beyond HEP, IDDS was adopted by LSST to manage large-scale data processing. Given the significant raw cost of disk storage – by some estimates, HL-LHC dedicated disk storage is more expensive than CPU – tight management of disk buffers has the opportunity to reduce their required size, allowing the community to rely more on less-expensive archival tiers.
Current and Potential Future Activities:

- Integration between IDDS and ServiceX: Currently the column delivery service (ServiceX) for analysis facilities is entirely dependent on the input datasets being on disk and being transferred then processed. By having ServiceX call out to IDDS to do the data processing, there's the opportunity to use this technology to stream datasets from tape into an analysis facility, extract columnar data needed for an analysis without needing to persist the entire dataset on disk.

Analysis Projects

Delivering columnar data with ServiceX

Funding Scenarios: Medium, High
Description: Columnar analysis is a relatively new and growing approach to physics analysis. ServiceX is an service designed to run inside analysis facilities to create and cache columns to meet analysts' data delivery needs. ServiceX was designed from the beginning to read experiment specific data formats and write selected events and properties to common columnar data formats used in industry (in addition to the HEP-native "ROOT" format).
Current and Potential Future Activities:

- Broaden the set of usable data formats: Analysis approaches are ever-evolving as the compute models for HL-LHC are refined. ServiceX has focused on the compact, analysis-oriented data format; however, new ML techniques often include the use of low-level objects that might be in more raw data (potentially on tape, needing IDDS integration). By building as broad a set of use cases as possible, ServiceX can help increase the impact of future analysis facilities.
- Integration with data management tools: The service can currently either deliver data to a S3-like object store; both provide quite simplistic tools for the management of data. When combined with industry techniques – for example, delivering to SkyHook (below) – there users will be able to better utilize those tools.
- Integrate with analysis preservation systems: One reason for the durability of "a dataset as a collection of files" is in its simplicity: the only data service needed to help reproduce a workflow is a filesystem. This is not necessarily true when a series of complex services is used to in the processing chain, including the case of delivering a column and integrating into into an existing dataset (which potentially implies the delivery service needs to be captured by the analysis preservation). To help sustain the ability to preserve analysis, commonly-used tools such as RECAST will need to understand/presserve analyses that were run with ServiceX.

Leveraging Industry Data Management for HEP

Funding Scenarios: Medium (reduced scope), High
Description: Analysis datasets will grow significantly *and* users will demand higher event rates to improve the time-to-insight. The Skyhook project is an investment into emerging data processing architectures where additional computational resources and hardware accelerators are available in the networking and storage layer. The service is leveraging commonly used data access libraries to "push down" structured queries into these layers to reduce data movement and to create views of datasets without creating copies. A significant part of the Skyhook project is the management of metadata that enables the establishment of views as well as versioning and branching of views (similar to versioning and branching in git-based source code management). Skyhook-enabled storage systems are a natural place for maintaining this metadata and servicing it to other tools in convenient formats. The project is leveraging data and query specifications of successful open-source projects such as Apache Arrow, Parquet, Substrait, and Apache Iceberg. The Skyhook project was able to upstream a Ceph extension to the Apache Arrow project, allowing Apache Arrow dataset interface queries to be pushed down and distributed into Ceph storage servers storing Parquet files. Other parts of the Skyhook project involve coordinated processing of Apache Arrow streams of particle physics data across multiple Bluefield SmartNICs using Substrait as query specification and processing status and offloading comparisons of genomes to hard drives.
Current and Potential Future Activities:

- *Integrate with file-based data management systems*: File-based data management systems like Apache Iceberg provide functionality typically associated with databases without losing the filesystem-based approach that LHC is heavily invested in. SkyHook is interested in utilizing the using ADL Benchmark library [57] as a way to compare Iceberg's performance with the to results presented by Graur et al. at VLDB'22 [58] and using py.iceberg as a mechanism to implement versioned views.
- *Alternate data modeling languages*: With such complex data as in LHC events, modeling and querying is not trivial and maps poorly to common languages like SQL; we aim to evaluate the new query and data modeling languages (such as Malloy) and compare it to results presented in [58].
- *Substrait integration*: Substrait is quickly becoming the established way to specify query plans independent of the original query language. It appears to be a promising way to create a composable data management stack that can unify multiple query approaches. For example, it would be able to help specify views and name cached queries and connect the LHC analysis stack to future data processing, management, and storage systems being developed in industry and wider CS R&D.

Joint Area Projects

Coffea-Casa, an Analysis Facility Platform for the HL-LHC (Joint with Analysis Systems, Facilities R&D)
Funding Scenarios: Medium, High
Description: One lesson learned from the first four years of IRIS-HEP is the difficulty in keeping multiple projects at different levels of maturity aligned toward a goal. Coffea-Casa is a prototype analysis facility which aims to be a common integration point for a broad set of technologies and provide them with a first exposure to a user base of analysts.

Coffea-Casa starts with a base of the "Coffea" processing framework for low latency columnar analysis and has a modular approach for adding other services such as ServiceX, SkyHook, or scale-out of tasks into a traditional batch system. The facility provides an interactive experience for physicists that's closer to working on a laptop as opposed to a traditional batch system-based facility. The facility adopts an approach that allows transforming existing computing facilities into composable systems using Kubernetes as the enabling technology. Kubernetes not only enables rapid deployment of services by developers via the DevOps methodology but also serves as a common language for service orchestration (see Section 5.5), enabling the services to be easily duplicated across multiple Coffea-Casa instances.

Within IRIS-HEP, Coffee-Casa is used to execute the exercises of the IRIS-HEP Analysis Grand Challenge (Section 6.1) and has deployments for the U.S. CMS & U.S. ATLAS physicist community.
Current and Potential Future Activities:

- *Maturing Coffea-Casa to production*: As the analysis facility concepts and services mature, we are working to expand the user base to help gain the experience necessary for at-scale analysis for the HL-LHC. We will continue to utilize Kubernetes as a technology fabric for additional services and enabling portability. Coffea-Casa will grow and scale along with the increasingly complex set of Analysis Grand Challenge exercises. The integrations with real CMS & ATLAS analyses will help us tune and benchmark for HL-LHC data rates. Further, as the prototype facilities scales from today's dozens of users to potentially hundreds, we expect challenges requiring improved resource management within these facilities.
- *Strengthening the integration across DOMA R&D*: As the integration point for analysis-oriented work in the IRIS-HEP Analysis Systems and DOMA areas, there is a continued need for Coffea-Casa to deploy new versions and data delivery services. Integrations with existing projects need to be strengthened (such as having ServiceX authentication credentials

be auto-generated on login or scaling data caching services) and starting integrations with new technologies such as bearer token support for authorizing global data access.

- *Develop approach for enabling ML-based analysis*: Machine learning techniques have a long history of use within HEP. However, they have rarely grown to the size where their needs need explicit planning in the site infrastructure; as ML rapidly grows across science and industry, the interest in the LHC community has grown as well. We will investigate approaches offering an interactive training environment with GPU access (more difficult than CPU scheduling as there are few GPU devices in the facilities) and pursue opportunities to integrate with national-scale GPU / ML training resources. Additionally, industry has built several new tools for deployment on Kubernetes – such as MLflow – to manage hyperparameter optimization tracking and advanced ML pipelines. Finally, multiple analyses have already begun to include ML inference into their workload; these would benefit from facility-local inference services to accelerate throughput.
- *Analysis preservation*: The addition of new service types (data management, ML inference services, task-based computing) creates new paradigms that need to be reflected in analysis preservation systems. Preservation strategies need to be devised and integrated with other community projects.
- *Coordinating the growing network of LHC analysis facilities*: IRIS-HEP is not the sole entity investigating analysis approaches for HL-LHC; there are several similar efforts globally. There's a role for a future software institute to serve as an intellectual hub, ensure coordination and knowledge sharing between international projects, NSF-funded efforts, and the U.S. LHC facilities.

> The prototype Coffea-Casa facility has proven to be a valuable "meeting point" for IRIS-HEP's analysis R&D vision and the team serves as an intellectual hub inside and outside the institute.

Core data streaming with XRootD and XCache (Joint with OSG-LHC)
Funding Scenarios: Medium, High
Description: The XRootD software framework is foundational for efforts across the LHC. It is used as a reference platform in IRIS-HEP for data streaming and bulk data transfer, as the basis for data federations in CMS, and, in its "XCache" configuration, as a data caching service for both production and analysis. Sustainability of this platform is essential.
Current and Potential Future Activities:

- *Evolving bulk data transfer*: As a multi-protocol server, XRootD implements both the proprietary "xrootd" protocol and the standard HTTPS. It is used by over half the U.S. LHC facilities for HTTP-based data transfer between sites. As the technology stack for bulk data transfer evolves – refining HTTP-based data movement, scaling the data rates, and implementing technology – this platform will continue to lead the community.
- *Core development, integration, and delivery*: Beyond bulk data transfer, XRootD is critical software for the LHC community. It is a collaboration with contributions from DOE labs, universities, and CERN; there is a role for the DOMA and OSG-LHC strategic areas to make contributions (core development, testing, integration, software delivery) to ensure the investments in this software are sustained. Having an institute-class investment from NSF like IRIS-HEP participate in these activities would help the collaboration provide a broader stakeholder setup for the NSF cyberinfrastructure community.
- *Exploring event delivery*: XRootD's multi-protocol framework includes an RPC and streaming layer which provides for a way to scalable, load-balanced data delivery. The SkyHook project

has shown the value of Apache Arrow as a high-performance, interoperable data format; however, it is currently limited to being used as part of Ceph (reasonably common, but nowhere near universal at LHC facilities). There is potential in using XRootD as a way to deliver high-level, structured data in Apache Arrow format while leveraging the existing authentication and streaming features of the software.

Impact and Success Criteria

DOMA has constituted a historical strength of the US university community. Particularly, in the last 5 years, the existing IRIS-HEP team has held leadership positions within the WLCG in this area and has designed and executed the transition from GridFTP to HTTP-TPC and began the transition to tokens. Investing in DOMA as part of an NSF-funded software institute would keep the HL-LHC community well-aligned with the activities and priorities of the broader NSF Office of Advanced Cyberinfrastructure (OAC); DOMA is uniquely situated to leverage existing distributed testbed resources in its program of work. Existing teams are in place for services like ServiceX and Skyhook and able to build on the success of the IRIS-HEP project. Having DOMA as a strategic area balances continuity – completing projects that will be in progress at the end of IRIS-HEP – with leveraging an existing productive team to start new projects. Further, the team will be able to help sustain critical projects such as XRootD widely used across the community.

The high-impact outcomes for the production activities in DOMA will revolve around the successful participation in, and execution of, the biennial data challenges coordinated in part with WLCG. The capstone of this effort will be the 2027 data challenge (approximately Year 4 of the next phase of IRIS-HEP) where we will aim to demonstrate bulk data transfers at 100% of the expected HL-LHC data rates. Another significant milestone will occur for DC23, when the majority of transfers will be run using token-based authorization. For DC25, we expect the remainder of the infrastructure will be token-based and the community will be leveraging from network services to improve accountability, monitoring, and management of data transfers.

For analysis-related activities, the expected outcomes of the DOMA strategic area will be around the usage of new paradigms of analysis facilities and the associated data delivery and management services. We expect these to be the most common analysis environment at the start of HL-LHC and for the Institute to demonstrate data rates to analyses at HL-LHC scale, as defined by the Analysis Grand challenge, by 2026. ServiceX is expected to be the primary way for users to ingest official experiment datasets into their analysis environments, Skyhook or similar services will provide a way to manage data (virtual views, joins of columns) from within the environment, and for analyses to have access to production-quality, user-facing services for ML inference.

HL-LHC Computing Gap Impact: The DOMA area is expected to make an impact on all four defined HL-LHC computing gaps. Most of the resources will be dedicated toward *G2 (Scalability)* as part of the benchmarking of different software components and the participation in regional data exercises and global data challenges. This work will provide a better understanding of our network flows and help increase the use of network services to increases the manageability of our data transfers translates on a more efficient use of our resources. The *G1 (Raw resource usage)* gap will be tackled through the investment in data delivery via IDDS which helps manage the disk buffers used for annual data (re-)processing and reduce the total amount of online disk needed for HL-LHC. For *G3 (Analysis at scale)*, DOMA will put new services and techniques in production a interactive facilities, combining “local laptop-like” responsiveness with datasets at the HL-LHC scale.

Finally, for *G4 (Sustainability)*, the DOMA area leverages industry protocols (HTTP, JWT-formatted bearer tokens), methodologies (Kubernetes-based service orchestration), and technologies (Apache Arrow) wherever possible. By helping the LHC community use broader ecosystems instead of developing technologies in-house, we minimize the LHC-specific pieces to those areas where the community is truly unique.

Success Criteria – Milestones & Deliverables:

The milestones and deliverables outlined below focus on the first three years of an Institute. These high-level items would be expanded and later years filled in as part of the execution of any project.

D4.1. Coffea-Casa used as part of one production analysis facilities in both ATLAS and CMS. **December 2023.**

D4.2. All the U.S. LHC T2s in the US support bearer tokens on their Storage Elements for Third Party Copy transfers. **December 2023**

D4.3. Rucio/SENSE integration is included as part of the DC23. **March 2024**

D4.4. Successful execution of DC23, meeting its data transfer and technology goals. **March 2024**

D4.5. ServiceX used for physics analyses as part of Coffea-Casa. **March 2024.**

D4.6. Demonstrate analyses running at 200Gbps as part of the Analysis Grand Challenge. **December 2024**

D4.7. Demonstrate the capability of XRootD to scale beyond 400Gbps. **June 2025**

Success Criteria – Metrics:

Metrics are a useful tool to provide management with quantitative insight about progress toward overarching goals. High-level metrics we expect to be applicable for the DOMA area are below:

M4.1. Demonstrate data rates as a percentage of the expected HL-LHC rates. Goals for this metric are defined by the DGC in the timelines set out in Section 6.2.

M4.2. Number of sites participating in the Rucio/SENSE testbed. Goal is 4 by DC23 and 8 by March 2025.

M4.3. Percentage of U.S. LHC facilities supporting bearer tokens for data transfer. Goal is $> 50\%$ as part of DC23 and for all sites by DC25.

M4.4. Maximum transfer rate demonstrated by the XRootD reference platform as a percentage of the desired HL-LHC rate for Tier-2s (400Gbps sustained). Goal is 200Gbps as part of DC23 and 400Gbps by DC25.

5.5 Facilities R&D and Integration

Facilities R&D broadly refers to activities related to the exploration and innovation of systems, services and physical infrastructure that provide platforms suitable for HL-LHC service environments and runtime ecosystems. These can be purely local facilities (platforms deployed within a local area network) or distributed, in the sense of interoperating services over wide area networks (the “Grid” or nowadays, distributed platforms). Two IRIS-HEP research areas (Analysis Systems and DOMA) have opted for software containers and cloud-native application management methods (Helm charts and GitOps) to standardize deployments. Driven primarily by DOMA software development and Analysis Grand Challenge scalability requirements, flexible strategies employing cloud-native technologies were tried out in the Scalable Systems Laboratory (SSL).

Indeed the concept of facility "substrates" using Kubernetes, a strategy pioneered in IRIS-HEP blueprint meetings, "k8s-hep meetups", and in WLCG Kubernetes workshops, are gaining popularity in production LHC analysis facilities as they offer reproducible application deployment and improved reliability of operation. The scope of facility R&D needed for the capabilities and scale of the HL-LHC, however, extends well beyond the substrate and includes several technological areas involving a diversity of data storage systems, innovative networks, and services for continuous integration and operation. Figure 10 illustrates the relationships between infrastructure, platforms and higher level services supporting production workflows.

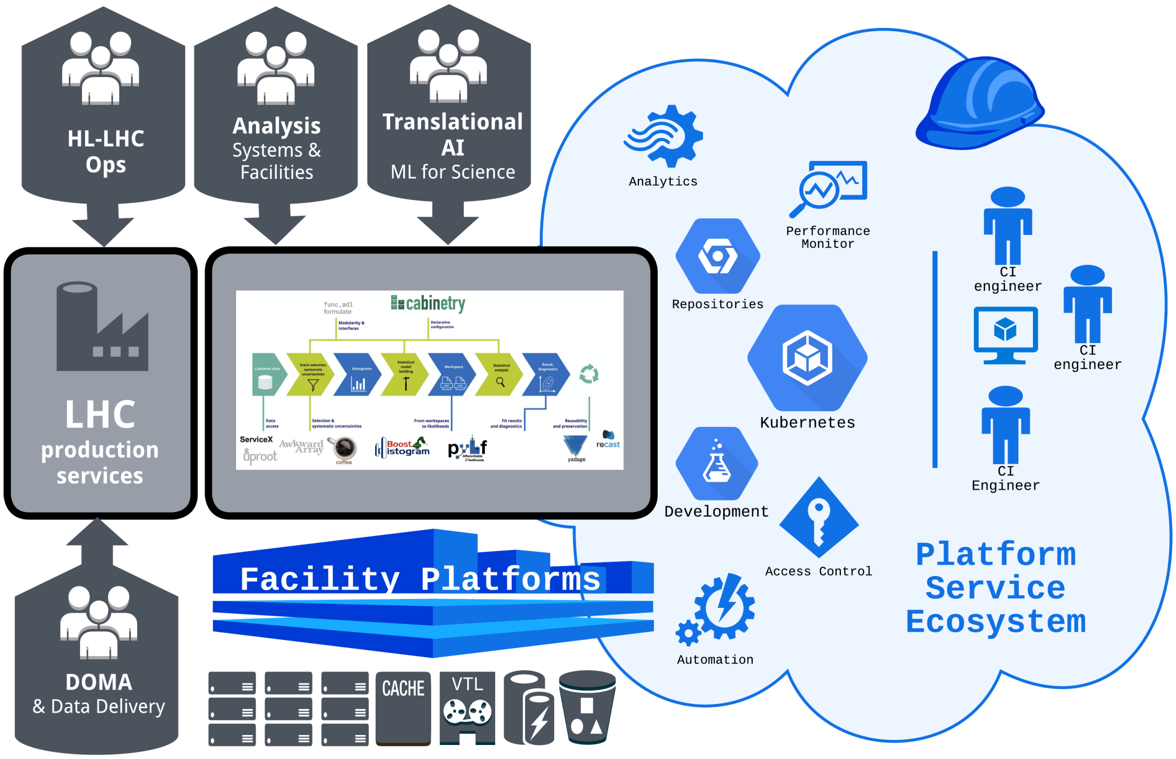

Figure 10: Schematic of illustrating role of Facilities R&D in the production and analysis ecosystem. CI engineers prepare and operate infrastructure and services in support of advanced data delivery, analysis, and other services.

Facilities Integration refers to activities relating to the installation, configuration, and operation of **development and pre-production** IRIS-HEP software components. Within IRIS-HEP these include Coffea-Casa, ServiceX, Skyhook, and other services. Other research cyberinfrastructure services finding application in the ecosystem (such as declarative processing frameworks, caching services, container image registries) likewise need to be integrated into production systems. Where possible development services are deployed in realistic contexts, alongside the experiment's existing systems and production infrastructure. This is the most immediate path to understanding which components in the overall cyberinfrastructure present the most significant scalability challenges. Collaboration between IRIS-HEP software developers and experienced U.S. LHC Tier-2 and Tier-3 systems administrators at universities is essential to achieve sustainable systems through the lifetime of the HL-LHC. This extends, as well, to distributed software developers in the US LHC Operations program as well as laboratory staff at the Tier-1 centers.

The IRIS-HEP Scalable Systems Laboratory is a Kubernetes DevOps platform for DOMA, Analysis Systems and Innovative Algorithms. The SSL hosts infrastructure for CoDaS-HEP training events and Analysis Grand Challenge pipeline testing and tutorials.

Specific Challenges and Opportunities

Over the past ten years, WLCG production computing infrastructure has remained largely static, managed with decades-old deployment and management techniques. Tier-1 and Tier-2 facility infrastructure, continuously in operation, has been able to cope with the event processing rates and storage requirements necessary to conduct the successful physics programs of the LHC experiments to date. This won't be true in the HL-LHC era unless those facilities change. For example, data access and delivery from distributed data sources to analysis platforms will require leveraging new capabilities in the network, in computational storage systems, in facility resource managers, and service orchestration frameworks. As we develop new capabilities to confront the data rates and processing scales of the HL-LHC, methods for infrastructure management and scaling become critical. The facility infrastructure itself must evolve.

This was recognized during the first phase of IRIS-HEP with the SSL providing two vital roles: a testbed infrastructure to incubate DOMA and analysis system prototypes to be evaluated by end-user physicists at LHC Run2 scales, and a challenge-environment for systems administrators and CI engineers to flexibly and adaptively create the needed infrastructure platforms. Already during LHC Run3, methods employed building the SSL have provided analysis facilities with a blueprint for infrastructure creation and operation. It is vital that SSL inspired facility R&D, together with pre-production service integration, continue during the next phase of IRIS-HEP. Considerable experience within IRIS-HEP and from integration with existing production services helps identify the near and longer-term challenges and opportunities for this area in the Institute.

Evolving Infrastructure for Next Generation Tier-2 and Analysis Facilities: Over the course of the next five years, the community will transform the historic roles of Tier-2 and end-user analysis facilities in the WLCG computing hierarchy to adapt to different sets of needs. For example, as opportunistic resources from leadership and national scale HPC centers are increasingly harnessed by the LHC experiments to fill the resource gaps (even during Run3 but more significantly for Run4), the Tier-2 centers, which currently are workhorses for centrally organized simulation and data derivation tasks, may increasingly become vital actors of the analysis and data delivery ecosystem. At present, they are not readily adaptable to take on those challenges. Similarly, end-stage physics analysis will shift from the laptop (or small-scale institutional clusters) to shared analysis facilities, hosting analysis and data access services capable of handling HL-LHC scale processing and data rates. Practically speaking, we may see these facilities blending roles and sharing responsibilities as frameworks for orchestrating services provide new agility for resources in the ecosystem.

To create, optimize, and reliably operate diverse services (such as analysis processing frameworks and data reformatting services) with sustained capabilities, and to ensure toolset adoption by the current Run3 physics groups, a sustained research and integration effort is essential. This will involve working at a nexus of disparate communities: LHC physicists, LHC (& HL-LHC) software developers, research cyberinfrastructure innovators, national and leadership HPC technical staff, the Research End User Group [59] in the Cloud Native Computing Foundation (CNCF) [60].

Distributed Infrastructure Management: DOMA systems intrinsically rely on distributed services to implement, for example, data delivery to analysis and production facilities. XCache networks deployed at multiple Tier-1 and Tier-2 sites for ATLAS and CMS are a prime example, essentially providing the equivalent of a commercial content delivery network (CDN) but with one important distinction: In the WLCG context, these services are mostly managed across administrative domains by multiple teams, leading to delays in software updates and in some cases inefficiency of operation. Lacking a seamless DevOps pipeline for the entire distributed platform, DOMA development teams are limited in their ability to advance new capabilities or respond quickly to bugs and security issues across the platform. Additionally, as analysis facilities scale to HL-LHC rates, we anticipate "scaling off-site" to handle bursty workloads during high periods of analysis activity. The off-site sources of processing cycles may come from Tier-2 production facilities, cloud resources, and potentially HPC centers (which are GPU-rich). A few groups have addressed this gap in capability through central management of services with techniques such as employed by NSF's National Research Platform (`https://nationalresearchplatform.org/`) which uses a single administrative domain (with full privileges) to combine resources from over 50 sites. In a similar manner, during the first five years of IRIS-HEP the SSL team partnered with the NSF SLATE project (`https://slateci.io/`) to develop a federated operations model ("FedOps") which requires only user privileges at Kubernetes-equipped clusters to deploy and operate edge services. With this approach an XCache network spanning all US ATLAS Tier-2 facilities, and extending to half a dozen more in Europe, are managed by one person allowing rapid updates as the underlying xrootd software evolves. During Run3 and LS3, the lead up period to HL-LHC, an opportunity exists to expand the number of services managed in this fashion, evolve the delivery tools with sustainable frameworks engineered with the broader CNCF community, and strengthen the operational policies and needed security models (work to be done with OSG-LHC).

Integration with Production Services during Run3: Software developed in the Institute eventually makes contact with the production ecosystem of the experiments and on production infrastructure. The sooner this happens the more quickly challenges are exposed and opportunities identified. To that end we've made certain that software graduated from the SSL that is ready for production deployment can have its entire lifecycle neatly packed up and reproduced elsewhere, such as at Tier-2s, national labs (Tier-1s), institutional clusters, HPC centers providing Kubernetes hosting platforms, and even within suitably equipped network testbeds (such as FABRIC). For example, ServiceX has been integrated with the production distributed data management service for ATLAS and CMS, essentially optimizing the data lookups, and exercised with production storage endpoints and production caches. Additionally, we have co-located the Coffea-Casa analysis facility software with shared Run3 analysis centers in production (both at Tier-2 and analysis facilities) to understand resource sharing, software access, identity management, data delivery, and user file system integration. The added bonus is side-by-side proximity to hundreds of physicists conducting analysis on data from LHC Run2 and Run3 thus simplifying the introduction of innovative capabilities from IRIS-HEP to new communities of users, gaining early feedback, increasing adoption.

Current Approaches and Development Roadmap

Facility R&D Across the Ecosystem

Funding Scenarios: High

Description: The Scalable Systems Laboratory is a unique resource in our field as it provides a flexible and diverse DevOps platform shared by IRIS-HEP software teams, developers from ATLAS and CMS, CI engineers from related NSF cyberinfrastructure projects, and LHC systems administrators. Part of its appeal is the context in which it sits, being (administratively) co-located with existing production LHC Tier-3 and Tier-2 facilities and infrastructure supporting a number of OSG-LHC related services (such as hosted compute entry points). It has proved to be an invalu-

able resource for not only IRIS-HEP software development and service deployment testing, but also a number of Kubernetes-deployable research cyberinfrastructure services including a network analytics service for WLCG PerfSONAR meshes, a network visualization service, an analytics service for ATLAS software and detector conditions data distribution, an XCache analytics service for CMS, scalability testing for FuncX (Functions-as-a-Service) by its core development team, a REANA test deployment, tests of containerized Rucio services, a notebook service for the annual CODAS-HEP training event, and a persistent notebook portal to GPU resources serving the ATLAS machine learning community.
Current and Potential Future Activities:

- *Continued operation of the reference SSL*: Providing a testbed infrastructure remains vital as IRIS-HEP software components continue to mature and operate with other services in the ecosystem. During the first five years of IRIS-HEP we established development and "production" SSL cluster testbeds to fit the cadence and stability requirements of the DOMA and Analysis Systems development teams. As these services come into production, this work will continue apace as developer sprints respond to user and operational feedback, new use cases and alternative strategies.
- *Constructing shared Tier-3 analysis facilities*: participate with the broader WLCG community in identifying best practices, infrastructure management patterns, and recipes forged on the SSL leading to reliable and scalable service deployments capable of supporting hundreds of users at Run3 scales in the near term, but with proven capabilities to scale up to Run4 during LS3.
- *Evolving Tier-2 infrastructure management*: retrofitting Tier-2 facilities with substrates and higher level infrastructure management tools and services, utilizing industry standard solutions where possible. The major focus will be placed on sustainability and key capabilities needed for stable, continuous Run3 operation while introducing new services targeted for HL-LHC demonstrators and challenge problems. Resources from across the Tier-2 complex will be needed in coordinated fashion for grand challenge scalability and other proof-of-concept demonstrators.

> The IRIS-HEP SSL informs the design of next generation WLCG Tier-2 centers and shared Tier-3 analysis facility infrastructure.

- *Capturing facility patterns and blueprints*: Creation and curation of GitOps charts and repository actions to provide reliability and reproducibility such that both infrastructure and applications can be easily replicated across facilities.
- *Identifying infrastructure (and service) bottlenecks*: a critical activity during data and analysis grand challenge exercises, and related demonstrator proof-of-concept exercises planned by the experiments, are load tests of representative software workloads that accurately mimic planned infrastructure and HL-LHC use cases. This will require instrumenting services and infrastructure with the needed monitoring hooks, streaming the resulting metrics to analytics dashboards, identifying and characterizing any bottlenecks that might exist, and measuring overall performance.
- *Exploring potential cost savings with ARM processors*: valuation and quantitative assessment of ARM processor technologies for HL-LHC will be a community-wide effort during the next few years. The US ATLAS Tier-1 will provide the ATLAS PanDA workload management system with an ARM testbed capable of testing a diverse set of simulation, reconstruction and analysis tasks. IRIS-HEP may leverage these resources to test performance and applicability for key services, for example ServiceX transformer performance on ARM. A related task

will be providing infrastructure for the OSG-LHC software team to build images for ARM processors and test needed variants of the OSG-LHC middleware (coordinated work with OSG-LHC).

- *Improve resource sharing across tasks on facilities*: It is well known that default resource allocation mechanisms offered by Kubernetes do not match the full spectrum of fair share scheduling capabilities for a diverse platform that may be simultaneously providing CPUs for ServiceX transformers, Dask workers for Coffea-Casa, HTCondor job slots for traditional batch processing. This must be dealt with during Run3 for shared Tier-3 analysis facilities which are providing new and old analysis environments.
- *Strategies for evolving storage system organization and access*: As described in the DOMA strategy above, a promising approach to accelerate access to data objects is to "push" a portion of the query evaluation down into the storage infrastructure, taking advantage of processors and potentially accelerators at that layer. Skyhook provides this capability for Ceph-based object storage systems. Measurements at scale scale and assessment of performance impacts for ServiceX transformers with Skyhook will need to be conducted for representative analysis queries and processing pipelines.
- *Future storage system R&D activities*: As described in the preceding DOMA strategy, closing the storage gap may indeed present the greatest computing challenge for the HL-LHC era. Over the next few years, efforts within IRIS-HEP and from across the LHC computing community will inform priorities for facility R&D activities in the Institute relating to promising storage technologies and approaches. For example, creation of heterogeneous storage systems for efficient analysis data access using distributed, asynchronous object stores (DAOS) and RNTuple formats will be explored in proof-of-concept exercises. Performance comparisons of processing rates with POSIX file systems over NVMe drives, distributed dCache pools with spinning disk (and accessed via xrootd protocol), and off-the-shelf object stores for both RNTuple and columnar data formats will provide valuable guidance to the community. The Institute will need to engage broadly and participate directly in specific demonstrators driven by the experiments.
- *Transparent storage quality of service and "tiered storage" models*: In many cases cost savings can be found if the expected workloads are better matched to the performance characteristics of the underlying storage systems. A transparent data quality-of-service that feeds this information to DOMA clients and to job workload management systems may achieve this. For example, a service which sends tiny log files to object stores, detector simulation input data to filesystems backed by spinning disk (very low I/O is required for those tasks), and analysis outputs to fast NVMe-backed file systems for speedy iterative access. Information collected would permit higher level services to move data to cold storage based on access patterns: very infrequently accessed data ("ice cold data") could migrate to machines programmatically switched off, something akin to Amazon Glacier, reducing overall facility costs. Facility managers would use analytics gathered in a given year to plan purchases for the following year, organizing procurement of storage types based on the experiment's projected needs by access category.

Managing Infrastructure over Wide Area Networks to Achieve Scale

Funding Scenarios: Medium, High

Description: Over the past several years significant advances have been made in remotely managing coordinated sets of services to more easily innovate systems while reducing operational cost. This has evolved our view of distributed computing resources from a cooperating grid of computing sites towards scalable research platforms offering programmatic capabilities for service orchestration, with dramatic potential impacts given the increased versatility of access. In the next phase of IRIS-HEP we anticipate making facility infrastructure advances for both data delivery and analysis processing incorporating these ideas.

Current and Potential Future Activities:

- *Reducing site storage requirements through caching*: Currently, both ATLAS and CMS employ data delivery methods involving differing access and caching architectures using XRootD technology which have direct implications on facility management and storage costs. Central tools for management of the global system can be used to introduce new capabilities and updates which strengthen the infrastructure. Current storage capacity requirements at WLCG processing sites can potentially be reduced using caches and knowledge of data placement and access history. Adding storage-less sites to the environment obviously would expand the pool of available CPUs and facilitate access to opportunistic resources. Additionally, existing WLCG sites with sufficient WAN bandwidth capacity could potentially retire their storage endpoints altogether and offer increased CPU capacity, trading storage costs (both operational labor and equipment) for additional CPU. As part of this activity we will stress-test caching networks with diverse analysis payloads at scale and provide performance and operational feedback to the DOMA development team.
- *Distributed workers to scale up analysis capacity*: Coffea-Casa analysis facilities to date have been deployed only on single-site, Tier-3 or Tier-2 clusters. For potential scale up to HL-LHC volumes, and to reduce waiting times on existing facilities in production, one could package and deploy lightweight service endpoints providing potentially an unlimited supply of Dask workers to a central home base (the "Casa"). Work is needed to understand the interplay and tradeoffs of providing centralized login servers, home servers, and local user storage services vs cloned stand-alone systems. The potential gains could be significant to reduce costs of analysis facilities (reducing their number) while vastly improving performance. Managing a coordinated network of lightweight worker providers, or "Coffea-Pots", across administrative domains is possible with FedOps techniques we've employed in the SSL.
- *Embedding advanced filtering services in the network*: We have begun exploring deployments of ServiceX inside the FABRIC testbed which opens up new strategies for data delivery and cost assessments in distributed environments. For example, by placing ServiceX on the server-side, at the data source, one can reduce bandwidth consumption between analysis clients and storage systems by combining filtering and reformatting functions at the source rather than copying complete files over the network. Significant impact could be made with implications for cost reductions of both network capacity and storage, both being expensive components of facility infrastructure. In Q2 2023, as part of the NSF FAB project (FABRIC Across Borders), a FABRIC "node" will be put into production at CERN, co-located with datasets hosted by the Tier-0. We will explore benefits of server-side ServiceX in operation at the Tier-0 while providing fast delivery of Run3 samples to production analysis facilities in the U.S. The exercise will provide an estimate of potential bandwidth reductions on the costly transatlantic link.
- *Upgrading the WLCG software distribution and detector conditions data caching network with modern software*: We have begun investigations of alternate approaches for managing cache-friendly data at WLCG sites, such as using the Varnish (`https://www.varnish-software.com/`) software. Alternate data distribution methods would aim to decrease the total cost to operate WLCG sites, helping close the overall resource gap.

Integration with Experiment Environments on Production Infrastructure

Funding Scenarios: High

Description: Throughout the development process, from prototypes to pre-production software and systems, there are points of integration with the larger software ecosystems of the experiments that must be designed, developed and iteratively tested. This requires significant and frequent contact among the development teams and with systems staff from the facilities. In addition, to perform meaningful tests with live environments and at meaningful scales for grand challenge demonstrators, production-scale resources must be marshalled and fair-share scheduled with on-going operations. *Current and Potential Future Activities*:

- *Facility integration of pre-production services*: In the first phase of IRIS-HEP, providing efficient interfaces between ServiceX and Rucio, the LHC data management service, was a significant challenge and required several optimizations to reduce latencies in queries to the central production service. As Rucio evolves with its own development roadmap this integration work will need to continue. As discussed in the DOMA strategic plan, integration of ServiceX with iDDS provides an opportunity to scale-up transformer processor capacity, and conversely, provide PanDA brokered analysis tasks with a columnar reformatting service. There are potential performance benefits from improved integration of ServiceX with XCache that can only be explored in production settings. Infrastructure and deployments for ancillary services like MinIO, the storage service for ServiceX formatted data outputs, including utilities to manage these outputs are needed. Discovering and removing experiment-specific dependencies (overlooked from early development prototypes) making them suitable for use by multiple experiments is often done in this phase. Supporting operation and user access to pre-production instances of DOMA services and analysis facilities for early adopting communities, including first draft user guides, requires expert knowledge from both domains.
- *Preparing demonstrator resources at scale*: Our approaches to date have been driven by IRIS-HEP developer priorities, analysis grand challenge goals, facility R&D opportunities, and a desire to find a sustainable path forward for creating declarative, reproducible cyberinfrastructure capable of scaling out to wherever resources may be found. In addition to IRIS-HEP data and analysis grand challenge exercises, the LHC experiments are planning additional demonstrators as input to computing technical design reports (TDRs). These TDRs will include a prioritization of R&D projects to complete during Long Shutdown 3 (S3) of the LHC. To inform those decisions, R&D projects for TDRs must provide a program of work towards the Run4 software and systems releases. They must include risks and effort estimates and proof-of-concept demonstrators which will lead to estimates on impacts for resource utilization (e.g. CPU time, GPU time, RAM, local disk and class of service, tape, and networks). IRIS-HEP will work with the computing and software management teams to align goals, configurations, data sets, and platforms to be used for these impact studies.
- *Advanced integration with HPC facilities*: Even as HPC resources are viewed as a prime opportunity to close the processing gap during the course of HL-LHC, coupling the experiment's data and workload management services to those facilities will remain a significant challenge as high energy physics is only one of a broad collection of science-drivers served by those facilities. A number of challenges have been identified in a recent workshop (`https://indico.cern.ch/event/1183995/`), among them data delivery into and from these facilities. HPCs are likely to support Kubernetes platforms within their infrastructure, even beyond edge platforms for hosting user services, potentially providing additional options to incorporate those resources into the LHC computing environment. Working with OSG-LHC, the SSL group will contribute to strategies to efficiently interface experiment systems with the resource "APIs" of HPC facilities.
- *Infrastructure for training and on-boarding*: To ensure community adoption and maximize user feedback to developers, it is essential to continue to provide training infrastructure for IRIS-HEP software tutorial events, experiment on-boarding events to analysis facilities, and advanced training activities sponsored by the Insitute, such as the annual Computational and Data Science Training for High Energy Physics school (CoDaS-HEP). Where experiment dedicated resources cannot be used (e.g. production Tier-3 analysis centers), the SSL can provide the necessary notebooks, CPU and GPU resources for diverse groups of young researchers

during these events.

Impact and Success Criteria

Equipping IRIS-HEP with the Scalable Systems Laboratory not only accelerated the pace of development of DOMA and Analysis Systems, and their integration with experiment production services and facility systems, but due to its versatility provided a unique resource in the field of high energy physics computing. The SSL has hosted instances of the ATLAS Distributed Computing Analytics Platform (`https://analytics.mwt2.org`), OSG Compute Entry points (providing access to cluster resources from over 20 universities), and provided a DevOps environment for a diverse community of CI engineers. Clearly the SSL facility and team assembled to operate it has been an important contributor to the overall NSF cyberinfrastructure ecosystem. The SSL implemented approaches for creating and managing flexible and reproducible infrastructure that others in the WLCG community are adopting. Maintaining an agile, open facility environment to incubate ideas, try out service prototypes in context, explore and cultivate new patterns for infrastructure delivery, and to confront the integration and scalability challenges over the next five years will be vital to the success of the Institute.

It is important to note that while specific resources (dedicated clusters) and infrastructure have been assembled and labeled as "the SSL" in the first five years of IRIS-HEP, facility R&D is of course broadly scoped and distributed across the community, receiving contributions from software developers, CI engineers, systems administrators and researchers from many universities, national laboratories and CERN. In the Institute we have the opportunity to bring convergence to approaches from many sources that will close the gaps to meeting HL-LHC computing resource needs and capabilities.

Success Criteria – Milestones & Deliverables:

As for other areas in an Institute, the milestones and deliverables outlined below focus on the first three years. These high-level items would be expanded in later years as part of the execution of any project. Note however that at the time of writing, many proof-of-concept demonstrators and facility R&D topics are being planned by the wider community during this time frame, potentially impacting deliverables described below.

D5.1. Establish infrastructure and orchestration services necessary for a sustained reference SSL. **December 2023**

D5.2. With DOMA, ServiceX deployed inside FABRIC at CERN. **December 2023**

D5.3. Releases of Analysis Systems pipelines supporting distributed analysis deployed on SSL. **Continuous**

D5.4. Provide a deployment package for upgraded software distribution and conditions data caching servers. **May 2024**

D5.5. With AS, evaluate distributed workers for Coffea-Casa. **May 2024**

D5.6. Curate and publish production Tier-3 deployment patterns including integration of traditional systems in use during Run3 and forward-looking analysis systems. **December 2024**

D5.7. With AS, support demonstration of running a full analysis suitable that uses machine learning. **December 2024**

D5.8. Evaluate technologies, services and infrastructure management patterns for next generation LHC Tier-2 facilities and publish for the community. **December 2025**

Success Criteria – Metrics:

Metrics are a useful tool to provide management with quantitative insight about progress toward overarching goals. High-level metrics we expect to be applicable for the Facility R&D and Integration area are below:

M5.1. Number of deployed analysis facilities in production operation. Goal is 6.

M5.2. Number of sites providing distributed workers to an analysis facility in production operation. Goal is 3.

M5.3. Number of storage-less sites in sustained production. Goal is 2.

M5.4. Number of sites with upgraded software distribution and detector conditions data caching servers in production. Goal is 7.

5.6 Fabric of distributed high-throughput computing services

The LHC depends on a global, distributed cyberinfrastructure to process, move, and store data and that infrastructure will need to evolve to meet the needs of the HL-LHC. The OSG Consortium provides the OSG Fabric of Services, a tightly-integrated set of services which provides for the cyberinfrastructure of the existing LHC experiments within the US.

> Established in 2005, the OSG Consortium operates a fabric of distributed High Throughput Computing (dHTC) services in support of the National Science & Engineering community. The research collaborations, campuses, national laboratories, and software providers that form the consortium are unified in their commitment to advance open science via these services.

The OSG Consortium is not a legal entity but a coordinated set of stakeholders working toward a common goal. A strategic area – the "OSG-LHC" - is needed to make contributions to the OSG Consortium to cover the existing cyberinfrastructure needs of the LHC, ensure the U.S. LHC facilities remain operational, and integrate the U.S. LHC facilities with the worldwide infrastructure.

Within the national distributed High Throughput Computing infrastructure, the LHC community leads in the scale and complexity of the distributed system. Through its participating in the broader OSG Consortium, work performed and knowledge gained for the LHC community has a broader impact than LHC and HEP. During IRIS-HEP, the OSG-LHC team has remained closely aligned with the Partnership to Advance Throughput Computing (PATh). The latter has a scope of all of NSF's Science and Engineering community, ensuring innovations done by OSG-LHC have a broad national footprint. The OSG-LHC helps the HL-LHC with both the scalability of its cyberinfrastructure and its sustainability by sharing it with multiple domains.

Over the past 15 years, the OSG Consortium has provided a stable foundation of software and common services to meet the HEP community's needs. An important aspect that is managing change in a rapidly changing world of software. For example, the OSG-LHC has led the transition of the entire national distributed high-throughput computing (dHTC) infrastructure from the niche "Grid Security Infrastructure" (GSI) identity-based authentication model to industry-standard bearer tokens implementing capabilities. When the Globus organization announced it would stop supporting the Globus Toolkit, the OSG-LHC team helped establish the Grid Community Forum and forked the toolkit to be the Grid Community Toolkit (GCT). During the first four years of IRIS-HEP, a major accomplishment was retiring the use of the GCT and replacing it with updated services.

OSG-LHC also integrates with rest of the institute. For example, through interaction with the Facilities R&D area, OSG-LHC began to add containers as a “first-class citizen” for software distribution; both DOMA and Analysis Systems groups make use of the OSG-LHC container registry; and DOMA’s work to implement bearer tokens or HTTP-TPC within the XRootD software is distributed in turn by OSG-LHC. Thus, software not only flows from the developers out to the communities but the ideas from within the institute also affect OSG-LHC’s approaches. Managing the full software lifecycle is a critical component of any distributed CI and an important role the OSG-LHC will continue to play in the future.

Specific Challenges and Opportunities

Rise of the container-native facilities Container-focused (“Cloud Native”) compute facilities are a generational change in how sites are operated and deliver capacity to the LHC experiments; see Section 5.5 for an overview of the rapid change in the cyberinfrastructure. OSG-LHC has significant expertise in delivering services as well-integrated software packages shipped in the operating system’s default packaging format. This historically was the desired mechanism for most sites that deploy the distributed services. Container-focused sites (largely deployed on top of Kubernetes) prefer services be delivered in containers, agnostic to the packaging or even the container OS, and have a higher-level service orchestration language for how services should be deployed. OSG-LHC has started to deliver services using these formats but there are still opportunities; for example, containers allow services to be delivered without needing superuser privileges on the host and container registries provide the ability to do daily scans of OSG-LHC containers for known security vulnerabilities.

Not all sites have an even adoption of newer technologies. There is a need amongst the cyberinfrastructure – not specific to any experiment – around Kubernetes community and knowledge building, including training and workforce development.

Increasing diversity of hardware resources The LHC community has long benefited from a period of relatively homogeneous resources – for well over a decade, all its pledged resources were x86 cores with 2GB of RAM. With the advent of GPUs, this has slowly started to change (although at a rate limited by the paucity of large-scale GPU workflows). The change to heterogeneous resources has a potential to accelerate as more ARM-based servers are released on the market an become competitive with capacity based on x86.

Integration with HPC, ML, and non-WLCG resources A common thread throughout the LHC lifetime is the fact its minimum hardware needs were met through its dedicated resources. During Run 2 and 3, additional HPC resources from outside WLCG were heavily utilized but these resources were never critical-path for the science program. For HL-LHC, to meet projected flat budgets, these non-WLCG resources will become essential. As part of its experiment-agnostic fabric, the OSG-LHC has the opportunity to help integrate NSF leadership class and ACCESS-allocated resources into the experiments’ fabrics.

A new type of resource and service expected for the HL-LHC will be machine learning inference services. Users have long used inference as part of their analysis but the complexity of the models are expected to increase rapidly through the years. Instead of trying to host sufficient resources within a LHC-specific facility, integration with a national-scale investment for inferencing would deliver value to the community.

Operating Production Services Unlike other strategic areas which have a mixture of projects in various stages of the software development lifecycle, OSG-LHC's purpose is to operate, maintain, and evolve production services. OSG-LHC must ensure the OSG Consortium's fabric of services remains operational and delivers value to the U.S. LHC Operations programs. This includes all parts of the lifecycle, including deprecation and obsolescence – for example, OSG-LHC will retire the OSG 3.6 software release series along with the June 2024 end-of-life of Enterprise Linux 7. OSG-LHC will help the community to bridge from today's cyberinfrastructure to HL-LHC's.

Current Approaches and Development Roadmap

Broadening Service Delivery

Funding Scenarios: Medium, High
Description: Services today are delivered as packages for the standard platform on the WLCG (Enterprise Linux 7, 8, or later on the x86 architecture). As the community progresses to the HL-LHC, the needs will become more heterogeneous (including ARM servers and the HPC platforms available as part of the NSF coordinated cyberinfrastructure in the next five years) and expect alternate delivery mechanisms (including container images and the service packaging such as Helm charts).
Current and Potential Future Activities:

- *Support for Heterogeneous Architectures*: Evolve the existing software compilations and repositories to also support non-x86 architectures including ARM.
- *Container-Native Service Delivery*: Beyond individual packages, create and maintain repositories of service descriptions for newer technology platforms like Kubernetes. Work with the community to develop and implement best practices such as reducing privileges inside the running containers.
- *HPC Integration*: The OSG-LHC has developed a variety mechanisms for integrating resources into the OSG Fabric of Services. This includes both the "Hosted CE", which integrates compute resources over SSH connections, and supporting XRootD endpoints on using unprivileged containers, giving access to storage resources at HPC centers.
- *Hosting Institute container images*: other areas of the Institute produce software outputs in the form of container images. Working closely with the Securing an Open and Trustworthy Ecosystem for Research Infrastructure and Applications (SOTERIA) project, OSG-LHC provides a national cyberinfrastructre-focused home for IRIS-HEP images.

Maintaining the OSG Fabric of Services

Funding Scenarios: Low, Medium, High
Description: Through the OSG-LHC, the OSG Consortium maintains services essential to the operations of the U.S. LHC facilities and their integration into the global cyberinfrastructure. Shared services include resource usage accounting, endpoint registration, and monitoring of service status.
Current and Potential Future Activities:

- *Packaging*: The OSG Software team, as part of the OSG-LHC contribution to the Consortium, maintains a curated software stack for facilities to use for services like compute Entrypoints (CEs), storage endpoints, and the worker node runtime client.
- *Resource and Service Registration*: OSG-LHC maintains an authoritative list of services part of the OSG Consortium and their association to administrators (necessary for communications and security responses). We aim to integrate with the CILogon-based Single Sign On (SSO) to ensure administrators can login to the infrastructure with their local credentials. The same

mechanisms can be extended to help simplify workflows for new Analysis Facilities and other services such as container registries for ATLAS analysis users.

- *International Cyberinfrastructure Integration*: Facilities have a requirement to report usage to the WLCG and report monitoring to ensure the U.S. LHC organizations are delivering on their commitments. OSG-LHC manages accounting and monitoring services and ensures they are adopted to changes coming from the WLCG.

Operational Cybersecurity
Funding Scenarios: Low, Medium, High
Description: Like any cyberinfrastructure, the LHC facilities, OSG Fabric of Services, and the user population are resources continuously targeted by hackers. The OSG Security area provides effort for operational security, responsible for security exercises and policy, responding to threats, and scanning services for vulnerabilities.
Current and Potential Future Activities:

- Coordination with global cybersecurity teams: Like data transfer, having functional cybersecurity requires interoperating with other infrastructures. The OSG-LHC cybersecurity team is the bridge between U.S. LHC efforts and EGI, CERN, and WLCG security teams.
- Improved monitoring of software artifacts and container-based services: Many of the security controls were designed when services consisted of packages deployed on physical hosts. The majority of services, however, run inside containers and are transient – meaning logs are likely lost unless they are retained inside a central logging service. Security controls need to be adopted and policies need to be updated to provide guidance to facilities on similar approaches.

Network Monitoring
Funding Scenarios: Medium, High
Description: Whether for bulk data movement or for streaming events to consumers, network performance is critical for the LHC community. The OSG-LHC Network Monitoring Area helps develop and operate technologies for monitoring performance and understanding network usage patterns at the application level.
Current and Potential Future Activities:

- *Packet monitoring*: Historically, network operators have had little insight into the usage of their networks by the LHC community which makes long-term planning more difficult. Typically, traffic between LHC sites are all labelled as "LHC" without regards to whether they are actually LHC traffic (versus other experiments), user versus production, or high priority versus low priority. The network monitoring team is working to have transfer services annotate packet header so network providers have richer metadata.
- *Leadership of the WLCG Network Monitoring task force*: Networking is another point where keeping the international community aligned is key. Currently, OSG-LHC co-leads the WLCG Network Monitoring task force and is well-positioned to guide network transitions between now and HL-LHC.

Impact and Success Criteria

OSG-LHC is unique among the Institute strategic areas in that its primary goal is to ensure smooth operations of the cyberinfrastructure for the LHC, with services meeting defined SLAs; "success" during this period is providing a operational roadmap to the HL-LHC era. However, there are expected outcomes and milestones beyond operations. For example, the area would finish the migration of services to Kubernetes and start supporting Kubernetes-only (or, at least, Kubernetes-centric) sites. The current OSG-LHC provides leadership in running production services on Kubernetes and we expect these new and converted facilities will rely heavily on its expertise. OSG-LHC will also be essential to the deployment of next-generation network monitoring, enabling network providers to introspect HL-LHC flows.

In its current incarnation, OSG-LHC consists of a team who have led the evolution of the OSG over the past 15 years, meaning there is a wealth of accumulated expertise in running a fabric of distributed high-throughput computing services and deep technical knowledge of how the current system operates. It is an essential element of any future Institute. Without it, the U.S. LHC operations programs would need to pick up the activities and it is unlikely that separate implementations by experiments would be as cost-effective as a common solution. Having the OSG-LHC be part of the future cyberinfrastructure for the HL-LHC will ensure key continuity of operations from now until the HL-LHC era.

HL-LHC Computing Challenge Impact : OSG-LHC will primarily have impact in the *G4 (Sustainability)* and *G2 (Scalability)* computing challenges. The approach of the OSG-LHC strategic area — contributing to the wider OSG Consortium -– improves the sustainability of the cyberinfrastructure by having a shared common layer across NSF Science and Engineering domains. We see this as being mutually beneficial: OSG-LHC will use the commons that have contributions from multiple projects and other projects will benefit from the unique scalability experience of the LHC/HL-LHC community. OSG-LHC will provide the foundational infrastructure for the HL-LHC and is thus responsible for ensuring the cyberinfrastructure can meet HL-LHC's scalability goals.

Success Criteria - Milestones:

D.1. Use of network flow monitoring as part of the next data challenge exercise; see Section 6.2. **March 2024**

D.2. Successful use of tokens for data transfers during the next data challenge exercise (joint with DOMA). **March 2024**

D.3. Retirement of the OSG 3.6 along with the end-of-life of RHEL7. **July 2024**

D.4. Remove last requirements and usage of GSI / X.509 security from the OSG Fabric of Services at the end of Run 3. **January 2026**

Success Criteria - Metrics:

M.1. Percent of critical OSG-LHC services meeting their agreed-upon SLAs. Goal is 100% of SLAs met, measured quarterly.

M.2. Number of IRIS-HEP and LHC container images hosted in the OSG-LHC container registry. Goal steady increase, measured quarterly.

5.7 Training and Workforce Development

People are the key to successful software. The community is currently building hardware upgrades and planning for an HL-LHC era which will *start* collecting data at the end of this decade, and then acquire data for at least another decade. People, working together, across disciplines and experiments, over several generations, will be the critical foundation underlying sustainable software.

Specific Challenges and Opportunities

Training support for software-related activities in HEP has historically been uneven. Although most universities do provide some relevant computer science and software engineering courses, and many now provide introductory “data science” courses, many HEP graduate students and postdocs are not required to take these classes as part of the curriculum. As students enter the research phase of graduate student training, many recognize the value of such classes, but are no longer in a position to take the classes easily. No “standard” recommendations exist for incoming students, either for HEP experiments or the HEP field as a whole. Some universities are developing curricula for STEM training in general or “certificate” programs for basic data science or software training, but these are by no means yet universal. The result has been that the graduate student and postdoc population historically had a diverse spectrum of relevant skills.

To address this, IRIS-HEP worked with HSF to develop a community vision five years ago (Figure 11) for a progression of training activities which, if implemented by the community, would create a new generation of software-enabled scientists. The ultimate goal was to invest today in the young students and postdocs who would become faculty leaders driving the research agenda in the HL-LHC era. IRIS-HEP has been working with the community to implement this vision. A sustainable framework for software training will be an important community legacy from IRIS-HEP and position the community to succeed maximally in the HL-LHC era.

Current Approaches and Development Roadmap

Basic Curriculum: Working with the HSF training group over the past few years, a complete basic curriculum (the lowest tier in Figure 11) has been implemented [61] at a level appropriate for HEP students. It includes material developed by The Carpentries and additional modules tailored to HEP beginners. Using this curriculum, the IRIS-HEP software training group and collaborators have organized more than 30 training events and trained over 1,500 students and postdocs. The material has also been adopted by the DUNE experiment for software training activities as well as the USCMS PURSUE summer student program [62], which focuses on broadening participation. Driven by a community of more than 50 motivated educators, the training modules are open-source and collaborative in nature. They span the spectrum from robust basic software skills to advanced topics like machine learning on GPUs. Sustainability has been the centerpiece of the approach, given that there are hundreds of new entrants in the community every year. Different tools and platforms, like GitHub, have enabled technical continuity, collaboration, and nurtured the sense to develop reproducible and reusable software. A significant effort has been devoted to ensuring that the basic software curriculum is taught frequently enough that most students can be trained very early in their research careers.

Following the approach of The Carpentries, each training module corresponds to a training webpage, including verbose descriptions, key-point summaries, and exercises to make training interactive. Recordings for all of our workshops are available, and several of our lessons are accompanied by dedicated videos targeting individual learners. As of 2022, the basic curriculum is considered complete and in production use by the community. A first set of reusable training modules on more advanced topics is also becoming available. (See Figure 12 for examples, and the HSF Training Center [63] for the full set.)

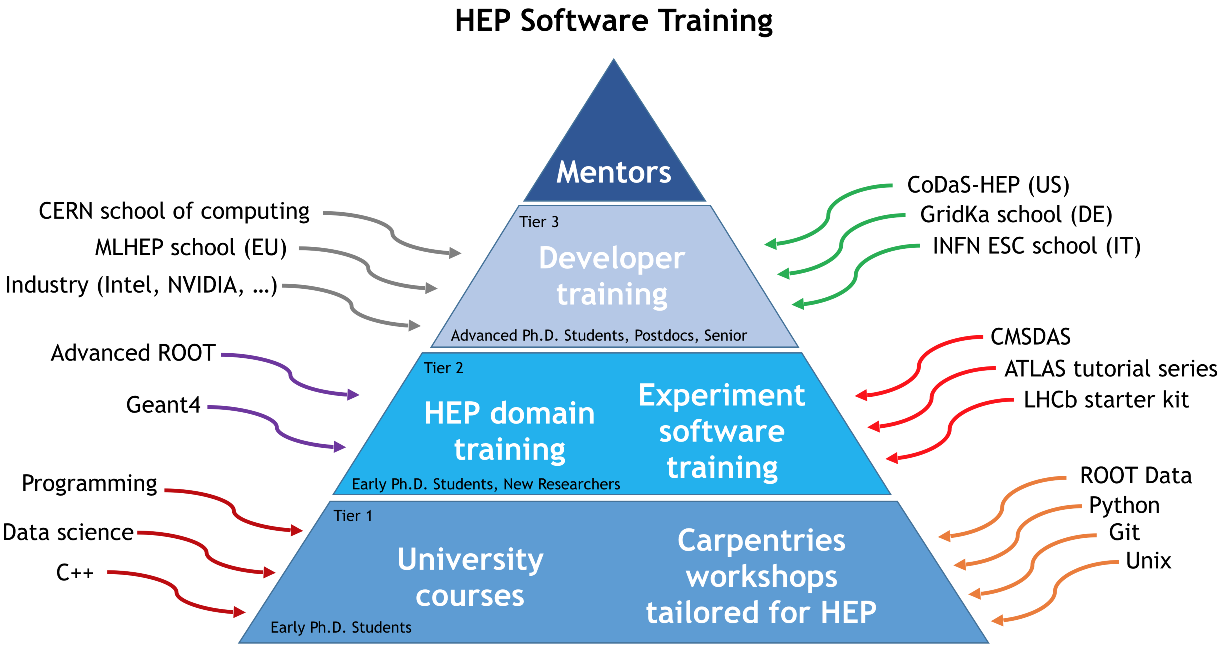

Figure 11: The HSF vision for software training in particle physics, from generally required basic software skills through advanced developer training, including eventual mentoring to contribute to research software projects.

Expert-level workshops and mentoring: While the basic training is typically sufficient for physicists involved primarily in small-group data analysis, many community members become Cyberinfrastructure professionals and will be involved in larger-scale software development activities for their experiments. Because of the long time scale of the experiments, imparting sustainable software development best practices is crucial. In addition, more advanced software and data science skills are often a strong asset when career evolution takes people to industry or other academic research domains. Offering orientation about different career paths for Cyberinfrastructure professionals will be an important aspect of sustaining the demand for software experts.

Some elements of more advanced training have been put in place. For example, the intensive week-long Computational and Data Science for High Energy Physics (CoDaS-HEP) summer school was begun in 2017 with the aim of teaching more advanced skills such as parallel programming, data science tools and techniques, machine learning technology and methods, code performance evaluation and collaborative use of git and GitHub. The school consists of both lectures and hands-on sessions and brings together young scientists from various HEP experiments (not only LHC) with experts from HEP and beyond. A “cohort” experience is also created by bringing the participants (that have similar interests) together in a single location for a week. The school was originally developed as part of an older NSF-funded project (PHY-1521042) and participant support has also been provided by an NSF CyberTraining award (OAC-1829729). Many instructors have, however, typically come from among the personnel funded by IRIS-HEP. The school was not run in 2020 and 2021 due to COVID, but began again in 2022 and is expected to run annually going forward.

Finally, it is important to note that many advanced concepts, such as architectural design decisions, cannot be easily imparted by teaching alone but must be practiced deliberately under

The modules

Basics

The UNIX Shell

A guide through the basics of the file systems and the shell.

Start learning now!

Contribute!

Version controlling with git

Track code changes, undo mistakes, collaborate. This module is a must.

Start learning now!

Contribute!

Programming with python

Get started with an incredibly popular programming language.

Start learning now!

Contribute!

SSH

Introduction to the Secure Shell (SSH)

⚠ Status: Early development

Start learning now!

Contribute!

Machine learning

Get behind the buzzword and teach machines to work for you intelligently!

Start learning now!
Watch the videos!

Contribute!

Matplotlib for HEP

Make science prettier with beautiful plots!

✱ Status: Beta testing

Start learning now!

Contribute!

`ROOT`

The most famous data analysis framework used in HEP.

Start learning now!

Contribute!

Software Development and Deployment

Version controlling with git

Track code changes, undo mistakes, collaborate. This module is a must.

Start learning now!

Contribute!

Advanced git

Learn to work with branches and more with this interactive webpage.

Start learning now!

Contribute!

CI/CD (gitlab)

Continuous integration and deployment with gitlab.

Start learning now!
Watch the videos!

Contribute!

CI/CD (github)

Continuous integration and deployment with github actions.

Start learning now!
Watch the videos!

Contribute!

Docker

Introduction to the docker container image system.

Start learning now!
Watch the videos!

Contribute!

Singularity

Introduction to containerization with Singularity/Apptainer.

⚠ Status: Early development

Start learning now!

Contribute!

Unit testing

Unit testing in python.

✱ Status: Beta testing

Start learning now!

Contribute!

Level up your python

Advanced bits of python (testing, debugging, logging, and more)

Start learning now!

Contribute!

Figure 12: Some elements of the HSF training curriculum. The full set can be found on the HSF Training Center website. [63]

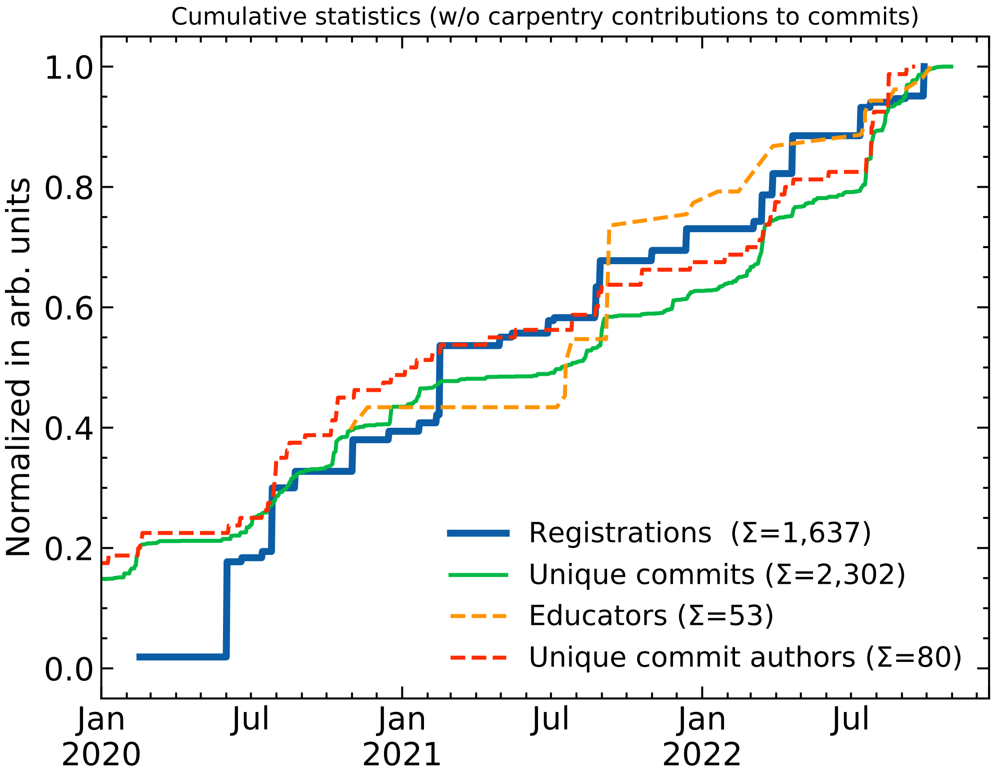

Figure 13: Growing the training group. Four different cumulative metrics are overlaid: the number of registrations in our events, the number of unique commits in our repositories (excluding commits to the framework developed by The Carpentries), the number of educators registered in the HSF Training community, and the number of unique commit authors (again excluding commits attributed to The Carpentries). The absolute values of each metric are shown in the legend.

Figure 14: Participants in the CoDaS-HEP 2022 summer school.

the guidance of mentors that have experience developing research software used by others. For this purpose, the IRIS-HEP Fellows program was created. Fellowships provide an intense and personalized form of developer training. During a period of several months, Fellows work on a project of their choosing, closely mentored by an expert from the field. By contributing to a HEP software project, Fellows obtain first-hand experience in collaborative software development and put their software knowledge into practice. Since 2019, more than 100 fellowships have been awarded. The success of the IRIS-HEP Fellows program funded by NSF has also attracted additional funding from private foundations and industry to extend the program. For example, twenty students from Ukraine were supported in 2022 and the Simon institute has supported around 5-8 international fellows every year since 2020. We see already that some of the CoDaS-HEP attendees and Fellows remain engaged with HEP research software development as they progress in their careers.

Plans for the next phase of IRIS-HEP: The current IRIS-HEP project has been instrumental in advancing the vision of a training pipeline shown in Figure 11. It is, however, not yet complete: in the HL-LHC era, we want every student entering our experiments to be fully conversant in basic software skills, with many possessing the more advanced software skills needed to create and evolve research software in HEP. Moreover, the available training progression will be widely recognized, and sustainability mechanisms will be established. For example, previous "students" of training activities may return as instructors for the next cohorts. The Fellows program will be widely recognized as an "on-ramp" for students to not only build skills, but also get connected to experiment and community research software activities. Finally, the students we train in the coming years include the faculty, staff scientists and research software engineers of the HL-LHC era.

5.8 LHCb & LHC Run 5

Lastly, we describe the additional strategic interest for ongoing collaborative efforts within IRIS-HEP regarding LHCb, another LHC experiment supported from the US primarily by the NSF. The upgrade plan for LHCb is out-of-phase with respect to ATLAS and CMS: major upgrades happened for LHC Run 3 and are planned for LHC Run 5. For example, between LHC Runs 2 and 3 LHCb underwent a major upgrade: its hardware trigger was removed and the first level trigger (Hlt1) now processes 30 MHz of beam crossings, about 5 TB/s of data. Extending several aspects of the software infrastructure will be important for LHCb in Run 4 and critical for Run 5, and may serve as models or starting points for software that is valuable to other experiments during the HL-LHC era.

As of Run 3, Hlt1 executes on GPUs with one instance of `Allen` [64] running on each GPU. Currently, every GPU receives complete events from an event building unit (an x86 CPU server) and handles several thousand events at once. Raw detector data is copied to the GPU, the full Hlt1 sequence is processed on the GPU; only selection decisions and objects used for the selections, such as tracks and primary vertices, are copied back to the CPU. The data rate between the two x86 server farms (the Hlt1 farm and the Hlt2 farm) is, therefore, reduced by a factor 30–60. `Allen` runs inside Gaudi in production. The native monitoring software inside `Allen` has an interface similar to that of Gaudi so the aggregated histograms are propagated back to the host, eventually giving them to Gaudi. In the future, LHCb plans to use Allen for the second level trigger as well. This requires additional work. An x86 compilation of Allen can run on the WLCG. In that case, the event loop is steered by Gaudi, and `Allen` is called one event at a time. While `Allen` is not the only approach to using GPUs for reconstruction and event selection entirely within GPUs, it demonstrates that this is possible. Other experiments might consider adopting it, or integrating some of its features into their GPU software. As GPUs become part of the WLCG, it will be important to build infrastructure to allow `Allen` to use these resources effectively. The environment will be very different from that of the online system, so the new infrastructure for using heterogeneous resources will take dedicated work. The same infrastructure could be designed to be common to all experiments using WLCG resources.

LHCb developed `PyConf`, to make Gaudi application configuration safer, cleaner, and simpler to debug. It was originally developed as a general pythonic functional framework for configuring complex CPU workflows, but it works for GPU workflows as well. At the moment, this package is specific to the LHCb version of Gaudi, but it should be possible to generalize for other users of Gaudi (such as ATLAS). This could be an appropriate effort for IRIS-HEP.

Recently, LHCb demonstrated that an `end-to-end` deep neural network (DNN) can provide better efficiency **and** a lower false positive rate for finding primary vertices (PVs) using simluated LHCb Run 3 data. It starts with track parameters and produces "target histograms" that a simple heuristic algorithm scans to extract PV positions and estimated longitudinal resolutions. Two separate DNNs are trained, then joined with extra channels added in the intermediate layer to allow the overall algorithm to learn additional additional details. The first consists of fully connected layers. It mimics the calculation of a heuristic kernel density estimator (KDE) that is a one-dimensional representation of where tracks intersect each other. The second is a convolutional neural network. It starts with KDEs and produces target histograms. Several CNN architectures produce statistically indistinguishable results. The preferred architecture is resembles the U-Net architecture [65] developed for image segmentation in medical applications. The `KDE-to-histograms` algorithm has been adapted to find PVs from simulated ATLAS data, and initial results are promising. Extending the LHCb algorithm to find secondary vertices and understanding how to best adapt the algorithm for use by ATLAS and CMS is a promising avenue for IRIS-HEP.

LHCb has deployed an older version of its `KDE-to-histograms` algorithm in its CPU software stack. Work is in progress now to deploy the full `end-to-end` algorithm inside `Allen`. NVIDIA's newest GPUs feature `tensor cores` in addition to `CUDA cores`. The former are optimized for the matrix multiplications that characterize DNN inference engines. On an RTX-A6000, they nominally provide 310 TFLOPS performance compared to the `CUDA cores`' 39 TFLOPS single precision performance. The `tensor cores` are not yet used by `Allen`. If the `end-to-end` inference engine can be run using the `tensor cores`, this will provide much better use of the silicon. A future direction for research will be studying how different DNN architectures most effectively use `tensor cores`. As many architectures can provide the same physics performance, identifying those that provide the best bang per buck will be important as we (HEP computing) think about how to replace other types of heuristic algorithms with DNNs.

A natural follow-on to developing DNNs to replace heuristic PV-finding algorithms is developing DNNs to replace aspects of Kalman filters. In an oversimplified picture, Kalman filters have three functions: (i) they describe trajectories, (ii) they describe the covariance matrices along the trajectories, and (iii) they provide quality metrics describing how well the hits used to construct the trajectories match the projected trajectories. In the same way that the algorithm for finding PVs was broken into two steps using domain expertise, the Kalman filter problem will need to be broken into steps and each step addressed separately before the pieces can be put back together again. DNNs do not need to provide better physics performance than heuristic algorithms – they need to execute more quickly by taking better advantage of the silicon available in GPUs. As the number of tracks per event increases during HL-LHC, this will become more and more important. While the details would change from one experiment to another, this is another area where a cross-experiment effort could produce a significant advance.

The work described in this section overlaps strongly with the work described in Sections 5.2 and 5.3. The `PyConf` work discussed in this section may help address some of the issues related to the increasing diversity of hardware resources in the WLCG discussed in Section 5.5.

6 Grand Challenges for the HL-LHC

Starting in 2020, IRIS-HEP has introduced the concept of a “Grand Challenge” within the institute to focus one or more areas on a long-term, large-scale goal part of the institute’s overall vision. A Grand Challenge differs from a more traditional milestone or deliverable by its scale (often requiring cross-cutting teams working together), a multi-year timeframe, and the fact the entirety of the approach may not be known upfront. The challenges are executed through a series of increasingly difficult exercises coordinated throughout the community. The currently defined grand challenges are:

- **Analysis Grand Challenge (AGC)**: The AGC aims to execute realistic analyses at the scale and complexity envisioned by the HL-LHC using a set of tools, facilities, and services developed within IRIS-HEP as an exemplar. The AGC team coordinates an annual workshop to demonstrate current progress against the goals and to update the vision and approach as necessary.
- **Data Grand Challenge (DGC)**: The DGC for IRIS-HEP is realized as a set of global data challenges coordinated with the WLCG. These challenges, occurring biennially, bring the entire global community together to demonstrate aggregate transfer data rates and compare what is currently achievable with the HL-LHC roadmap. These challenges also provide an opportunity for integrating new technologies being worked on by DOMA into the production infrastructure.
- **Training Grand Challenge (TGC)**: To tackle the challenges of the HL-LHC, we need a workforce with broad software knowledge, spanning from basic programming skills to highly specialized training. The TGC defines a roadmap to efficiently scale up training activities and provide adequate training to create the software-skilled workforce that will realize HL-LHC science.

Not every activity within the Institute fits into the Grand Challenge format. For example, the data reconstruction and tracking activities of each experiment are coordinated independently and, based on the differences in experiment timelines and production code, is not conducive to joint exercises. Instead, progress is typically tracked through improved relative performance and delivery to the experiments’ production frameworks.

6.1 Analysis Grand Challenge

> Physics analysis pipelines make use of a large number of tools and services — the Analysis Grand Challenge provides the mandatory end-to-end tests capturing the full complexity of workflows to ensure readiness of the stack for the HL-LHC.

The HL-LHC will be a challenging analysis environment compared to the LHC experiments of today. The data volumes will go up by a factor $\sim$100 and, to reach the desired physics reach of results, analysts will need new techniques and approaches as discussed in Section 3.3. What might be done on a laptop today with events stored on the local file system will need to be done on a dedicated facility in the HL-LHC era, leveraging large-scale computing hardware, advanced data delivery services, and ML training and inference environments. As described in Section 5.1, new tools and services are being actively developed to address these challenges.

Even if all the tools and services needed existed independently, their full potential can only be realized through integration into a coherent stack tuned to run on an Analysis Facility. The Analysis

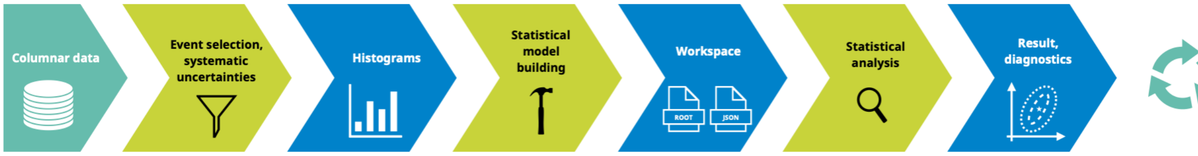

Figure 15: Data analysis pipeline for the AGC. This is a simplified view of the Analysis Systems pipeline in figure 8.

Grand Challenge (AGC) is designed to function as a series of escalating integration exercises with the ultimate goal of showcasing HL-LHC analyses at full scale and complexity. AGC brings together tools from the AS, DOMA, and Facilities R&D areas (and elsewhere) and defines physics analysis tasks, representative of the requirements of the HL-LHC, which have to be addressed with an end-to-end analysis pipeline that requires all the ingredients to work together effectively as a system. Figure 15 depicts the steps in analysis and by extension the components in the software stack.

The AGC connects not only to areas inside the Institute but also connects to the broader surrounding ecosystem; for example, the Coffea analysis framework used by the AGC has originally been developed by Fermilab scientists. The tools being built within and outside IRIS-HEP are designed as small pluggable libraries and steps in a toolchain rather than a framework. The AGC takes advantage of this by pulling in other tools where they are already developed.

A goal of IRIS-HEP is to help democratize science: anyone, associated with an experiment or not, can re-implement analysis pipelines with the tools and workflows of their choice. This allows the AGC to serve as a central gathering point for a larger community focused on end-user analysis in HEP. All the AGC demos and workbooks are openly accessible, and we strive to have as many components as possible based on publicly available Open Data so that anyone can try them out. At the same time, realism requires some demos are developed that run with the experiment's data.

The AGC will be executed as a series of annual 3-day workshops; each workshop will have a set of technical capability and scale goals set by the AGC leads. The exercises will be cumulative, building on the scale, complexity, and realism that was shown the prior year. The typical workshop will have one day of demonstrations from the IRIS-HEP team, one day of tutorials (splitting into ATLAS / CMS sessions if needed to talk about proprietary analysis techniques), and ending with a day of planning where the goals for the next workshops are set and updated.

Following the success of the AGC during the first phase of IRIS-HEP, there are opportunities for extending these exercises through the start of the HL-LHC. We expect that the AGC will continue to provide a platform for coordinated efforts and to organize information exchanges between different areas, programs, and other entities (e.g., ROOT project, CERN IT, Coffea). The AGC will function as an integration exercise and testbed for the latest developments, leading the analysis approaches into the HL-LHC era.

Existing work on the AGC

During the first phase of IRIS-HEP, the AGC selected as a pathfinder analysis a relatively-simple physics analysis task based on a $t\bar{t}$ cross-section measurement with CMS Open Data. IRIS-HEP implemented analysis pipelines heavily based on the Python data science ecosystem (including and complemented with analysis tools developed by the Analysis Systems area). These made use of novel data delivery methods such as ServiceX and exploited new services in analysis facilities such as Coffea-Casa. Starting from centrally-provided Open Data samples at CERN, the AGC implements the common workflow items relevant to data analysis performed by physicists for this analysis: data extraction and filtering, object calibration and evaluation of systematic uncertainties, construction of observables, histogramming, construction of statistical models and inference, and visualizations to study and disseminate analysis details and results.

IRIS-HEP demonstrated the feasibility of its analysis systems approach at dedicated annual AGC workshops [66, 67] and through contributions to relevant HEP conferences, such as International Conference on High Energy Physics (ICHEP 2022) [68] and International Workshop on Advanced Computing and Analysis Techniques in Physics Research (ACAT 2022) [69].

Annual AGC workshops dedicated to showcasing tools and workflows related to the AGC analysis pipeline included:

- **AGC Tools 2021 Workshop I**: The idea for the first AGC workshop was to introduce to end-users the various tools and services, as the components of an AGC analysis pipeline. These tools were developed in the Python ecosystem by and for the particle physics community as well and deployed on related cyberinfrastructure to be executed at scale. The workshop agenda also included specific experiment sessions to collect early feedback about pipeline and deployment from CMS and ATLAS analysts.
- **AGC Tools 2022 Workshop II**: The agenda of the second AGC workshop featured detailed hands-on tutorials based on AGC tools as well as providing the possibility for participants to follow all tutorials on dedicated Analysis Facilities provided by SSL (Coffea-Casa analysis facilities at University of Nebraska-Lincoln and University of Chicago).

These forums allowed the team to discuss the physics analysis workflow vision developed in the AGC with the community and to demonstrate the pipelines in practice. Tests of pipelines at scale at various analysis facilities revealed performance bottlenecks and usability issues which have subsequently been addressed. Different analysis pipeline implementations have been contributed, including a version using ROOT's RDataFrame, allowing the comparison of possible approaches available to users for physics analysis.

Next Phase of the AGC

We have found the annual workshops showing increasing scale, complexity, and realism of HL-LHC analysis to be a useful structure for accomplishing the AGC's goals and plan to continue these in the future. This subsection provides an overview for how the AGC plans to integate with various areas internally followed by the plans and goals for the next phase of IRIS-HEP.

Given the wide variety of physics analyses within the LHC community, for the next phase of IRIS-HEP we have selected two HL-LHC analyses as flagship examples to complement the current pathfinder $t\bar{t}$ cross-section analysis.

- **Top quark mass**: The top quark mass measurement in the $t\bar{t} \rightarrow \text{lepton} + \text{jets}$ channel is expected to require an extremely large analysis dataset due to the significant backgrounds in this channel. This will serve as a **high-volume** analysis that pushes the system's limits in terms of event rate.
- **Di-Higgs search**: The di-Higgs analysis program at the LHC probes the Higgs self-coupling, which is believed to be *just* within the reach of the HL-LHC dataset. Maximizing sensitivity to the trilinear Higgs coupling implies the use of the latest available ML and statistics techniques; the software developed by the AS area is meant to enable these approaches. This will serve as a **high-complexity** analysis example to bring together these tools.

Connections to Analysis Systems Unsurprisingly, there are many deep connections between the AGC and the Analysis Systems (AS) area; indeed, the AS team is the primary provider of tooling for the AGC exercises. Community interactions during AGC workshops proved to be a useful way to understand user experiences for analysis work. Based on these experiences and the remaining incomplete items from the overall vision, topics of work planned for the next phase of IRIS-HEP include:

- **Handling Systematic Uncertainties**: The handling of systematic uncertainties in an analysis pipeline was outlined as the top pain point for end-users in the Analysis Ecosystem Workshop II workshop report [70]. The AGC analysis tasks capture all relevant types of systematic uncertainties and the associated metadata handling to probe the associated user experience. The top quark mass measurement in particular is an ideal environment for this: dominant contributions limiting the sensitivity come from sources of systematic uncertainty, and a rich set of different types of uncertainties needs to be evaluated.
- **ML Services**: Integration of machine learning into the AGC framework has been a frequently requested item in community interactions. ML is increasingly commonplace in physics analysis but users often have to split ML training into a separate pipeline. The AGC can be used to investigate workflows that streamline the user experience, including identifying services facilities should provide to help with this.
- **Differentiable Analysis**: A differentiable analysis pipeline would allow for end-to-end analysis optimization via gradient descent, increasing the overall physics reach of the analysis. To accomplish this goal, all the different parts of the analysis pipeline need to support evaluating and passing gradient information along. The AGC can be used to track the progress towards increasing the number of pieces that provide the required technical capability and to test the functionality in a realistic environment.

Connections to DOMA The DOMA team contributes important data delivery services (capabilities) and expertise on scaling up data rates on the facilities used by the AGC (capacity). Topics that will be emphasized for the next phase include:

- **Data Delivery**: The data extraction and data delivery edge service, ServiceX, is providing data access functionality for the pipeline. It allows users to filter events, add additional columns to an event (for example, CMS NanoAOD) on-demand, and have the result placed at the facility. The target workflow for the next phase will be to allow users to select columns from NanoAODs, using the desired selection to skim and extract a column from MiniAOD files centrally, and finally retrieving the new column for the selection and integrating it back into the existing NanoAOD workflow. An analogous capability is planned for ATLAS datasets as well.
- **Data Management**: A critical capability for HL-LHC analysis will be to manipulate, augment, and subset data in-place without having to create a derived copy of the dataset (as is frequently done for the LHC). As discussed in Section 5.4, the next phase of the Skyhook project will be to allow joining together data from derived columns (in formats such as NanoAOD or PHYSLITE) used by analyzers with new generated columns or columns derived from the reference dataset (in formats such as MiniAOD or PHYS) as delivered by ServiceX.

Connections to Facilities R&D The third key component for the success of AGC is the investigation of modern cyberinfrastructure approaches that can compose these services into a facility, and to allow duplicating it to several locations. The AGC will work closely with the Facilities R&D area and other facilities, such as Fermilab and BNL, to provide a complex “in-house” use case demonstrating the needs of a modern facility.

- **Coffea-Casa Facility**: The prototype facility heavily used by the AGC is the Coffea-Casa analysis facility, developed as a cross-cutting project in IRIS-HEP that brings new, interactive paradigms for users from R&D into production. This facility is used as a testbed, offering the possibility for end-users to execute analysis at HL-LHC-scale data rates. It uses an approach that allows it to transform existing facilities (e.g., U.S. LHC T2 sites) into composable systems using Kubernetes as the enabling technology.

- **Scale**: We will extend the AGC input datasets to 200 TB to enable testing the I/O performance of analysis pipelines at a scale that is interesting to the cyberinfrastructure (this is about 20x larger than what is commonly used today for end-stage analysis). One component of each workshop will be to achieve certain processing time targets with this input dataset. Between workshops, the AGC will perform periodic benchmarking exercises on various partner facilities to ensure that no regressions appear when executing the pipeline at scale and with larger computation complexity.
- **ML Services**: The AGC will work to integrate emergent functionalities and services required by the analysis community such as making Machine Learning (ML) more readily accessible to users. We aim to include a ML inference server (one of the existing examples is SONIC [71]), built on NVIDIA's Triton Inference server, as a way to have transparent access to high-speed, GPU-based inference as part of user applications. The environment will be extended to include tools like MLFlow to help tracking user experiments with AI training. Where possible, the focus will be to integrate national-scale AI resources instead of only those internal to HEP facilities.

AGC Targets The AGC's annual workshop format allows us to have specific targets toward a full-scale HL-LHC analysis. The first AGC workshop of a possible next phase to IRIS-HEP would be in 2024; while there's an understanding of the volume and scale targets throughout the entire phase, it is more difficult to map out the precise ordering of new technologies this timescale. Table 3 outlines the possible goals and targets for the AGC.

Year	Target
2024	• Define analysis tasks for the top quark mass and di-Higgs measurement. • High-volume analysis done on dataset 20% the scale needed for HL-LHC and completed within 1 hour. • Integrate ML inference service with AGC.
2025	• High-volume analysis done on dataset 40% the scale needed for HL-LHC and completed within 1 hour. • Demonstrate AOD column extraction workflow
2026	• High-volume analysis done on dataset 60% the scale needed for HL-LHC and completed within 1 hour. • Demonstrate fully differentiable analysis
2027	• High-volume analysis done on dataset 80% the scale needed for HL-LHC and completed within 1 hour.
2028	• High-volume analysis done on dataset 100% the scale needed for HL-LHC and completed within 1 hour.

Table 3: Targets by year for the AGC in a five-year timespan.

6.2 Data Grand Challenge

> The data challenges are the global community's mechanism to prepare the cyberinfrastructure for the HL-LHC data rates and a mechanism for IRIS-HEP to ready new technologies for the production infrastructure.

HL-LHC has multiple challenges around data organization, management, and access. Perhaps too often, the 'data issue' in the HL-LHC focuses on the raw volume of data; however, it's insufficient to simply purchase a certain volume of hard drives. The problems also include *data velocity* – raw data must be moved from the detector to distributed sites, from simulation site to archival, and from buffers to HPC resources - and data management. For coordination of the distributed cyberinfrastructure, the data velocity is the more vexing issue as the data must be moved over shared network resources (implying coordination and resource management with multiple providers) and the technology stacks select must be interoperable with a global set of facilities.

Considering the datasets involved, the velocity – the global aggregate terabits per second – is also a scaling issue. The HL-LHC community will need to **sustain data rates 20 times larger** than the baseline set by LHC Run 3.

Simply put, the LHC community is not ready for the HL-LHC rates and the preparation is not solely a function of buying switches and fiber immediately before the accelerator turns on. Instead, a robust R&D program is needed in this area as outlined in Section 5.4, introducing new technologies into the software stack and demonstrating components' readiness for HL-LHC data rates.

To help integrate the global R&D efforts and show progress toward the ultimate HL-LHC goals, the LHC community has defined a Data Grand Challenge, a series of biennial exercises for data movement. These exercises have global sustained data movement targets as outlined in Table 4. Each exercise has two targets – the "minimal scenario" and "flexible scenario". The minimal scenario is derived from the input parameters from the computing models – number of events expected per year, size of each event format, and the minimum number of times a dataset needs to be transferred or processing. The flexible scenario is based on the experience of how LHC operates – data transfers are bursty and not flat over the year, we may need to move data to HPC resources to take advantage of large time-limited allocations, and data sometimes needs to be transferred for processing multiple times to account for software errors.

Year	Percent of HL-LHC Scale	Minimal Scenario Agg. Targets (Gbps)	Flexible Scenario Agg. Targets (Gbps)
2021	10%	480	960
2023	30%	1,440	2,880
2025	60%	2,880	5,760
2027	100%	4,800	9,600

Table 4: The aggregate global targets for the biennial data challenges as presented to the WLCG Management Board in February 2021 [17].

Each experiment's draft computing model provides a rough partitioning of data to different computing sites for HL-LHC; this is reproduced in Table 5. The global experiments' plans do not forecast at the Tier-2 level but the U.S. LHC programs have also participated in a network capacity planning exercise with ESNet [18] which additionally concluded that a **nominal Tier-2 site will need 400Gbps capacity** for HL-LHC.

LHC Tier-1 Site	HL-LHC Network Needs (Gbps) Minimal Scenario	HL-LHC Network Needs (Gbps) Flexible Scenario
CA-TRIUMF	200	400
DE-KIT	600	1,200
ES-PIC	200	400
FR-CCIN2P3	570	1,140
IT-INFN-CNAF	60	1,380
KR-KISTI-GSDC	50	100
NDGF	140	280
NL-T1	180	360
NRC-KI-T1	120	240
UK-T1-RAL	610	1,220
RU-JINR-T1	200	400
US-T1-BNL	450	900
US-FNAL-CMS	800	1,600
(Atlantic Link)	1,250	2,500
SUM	**4,810**	**9,620**

Table 5: The breakdown of expected data rates per site as presented to the WLCG Management Board in February 2021 [17] for the purposes of planning the data challenge exercises.

Existing work on the DGC

The inaugural data challenge, DC21, had a target of 10% HL-LHC scale. This target is similar to the current production scale for LHC Run 3 meaning the challenge largely focused on (a) building a reusable infrastructure necessary for running this and future data challenges, (b) demonstrating the ability of the global community to collaborate on such a challenge, and (c) prove new technologies at production scale.

There were two important new technologies for DC21:

- **HTTP-TPC**: A majority of transfers were made with WebDAV-based HTTP-TPC protocol. HTTP-TPC is an agreed-upon interpretation of the WebDAV protocol that is built on industry-standard HTTPS. After the data challenge, the experiments officially committed to using HTTP-TPC in production for LHC Run 3; this represents the first upgrade in transport protocols in two decades and the only change in protocol since the start off LHC Run 1. Using HTTPS as a base reflects evolutions in the wider industry, and keeps the LHC community on a **sustainable path for the future**.
- **SRM/HTTP**: The tape / archive management protocol used by the WLCG is Storage Resource Management (SRM) protocol. SRM utilizes a proprietary TLS-like transport layer with SOAP as the RPC layer; neither technology is widely used in modern environments. Further, SRM is based upon a model of remote space management that has been discarded by the WLCG – only the small subset of the protocol (tape management) is used. The LHC cyberinfrastructure is in the middle of replacing this dead-end technology; the first step was during DC21 where, instead of layering SRM on top of GridFTP, HTTP-TPC was used.

DC21 successfully executed all its goals. The exercise was held in October 2021, performed using the same Rucio / FTS software stack used in production by ATLAS and CMS, and hit the target data rates for both the minimal and flexible scenarios.

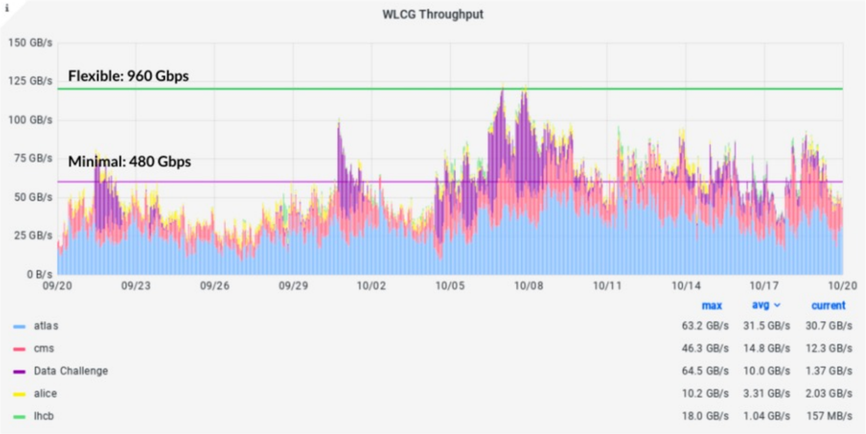

Figure 1 - Mock DC1 22/09/2021; Mock DC2 01/10/2021; Network Challenge (DC) 04-10/10/2021; Tape Challenge 11-19/10/2021.

Figure 16: The hourly average data rates achieved by successful transfers during DC21. Figure is reproduced from the report at [72].

Next Phase of the DGC

In the next phase of IRIS-HEP, we will participate in the next four data challenges. Below, we outline the known plans for the next challenge - DC23 (due to scheduling conflicts, currently planned for March 2024) - and subsequent exercise.

DC23: DC21 validated the approach of executing coordinated data movement exercises for the Data Grand Challenge. The next data challenge, DC23, is more difficult as it has both a robust "new technology" component and serious scale challenges, tripling the target data rates from 10% to 30% of HL-LHC scale (the largest relative increase in the DGC program). Planned new technologies and capabilities for DC23 include:

- *Dynamic engineered network paths*: Using technologies provided by ESNet, show the ability to migrate specific flows to dynamically engineered paths, associating the traffic type with a specific path enabling the ability to do differentiation in the future.
- *New authorization paradigm*: The U.S. LHC computing facilities have already transitioned from identity-mapping based authorization to capability-based, providing a fine-grained approach to authorization. The equivalent change for data transfers is underway and expected to be a cornerstone for DC23.
- *Emphasis on IPv6*: IPv6 is becoming widely deployed across the WLCG and is a prerequisite for new network technologies. Its header extensions are used for adding metadata to network flows, enabling improved monitoring of flows outside of engineered network paths. We aim to have a majority of transfers use IPv6 during DC23.

Additionally, the U.S. LHC community is investigating regional mini-challenges to ensure that its facilities are prepared for the increased data rates. For more information on the technologies involved, see Section 5.4.

Post-DC23: The precise set of technologies that will be ready to integrate into production in 2025 and 2027 are less clear. Given DC21 and DC23 represent a generational change of transfer protocols and authorization approaches, the expected focus for DC25 and DC27 will be increasing the scale of the production system. Software scaling tests, with some efforts starting already, will be critical to get the storage endpoints ready for these challenges; DC25's target data rates will be an order of magnitude larger than today's production traffic. Post-DC23, production facilities will start the purchase ramp-up of hardware, allowing the community to rely more on production endpoints over testbed facilities.

6.3 Training Grand Challenge

The science of the HL-LHC will be highly software-enabled. Maximizing the physics output requires that community members from all career levels have a solid base of knowledge in order to leverage the software tools being developed. Even for small group collaborations or single individuals developing a physics analysis, software literacy is fundamental. For this category of "Cyberinfrastructure Users", training should include basic programming, version control, best practices of state-of-the-art software engineering, etc. A large subset of the community will then also be involved in developing software tools that will be used by their collaborators and perhaps contributing to the community ecosystem ("Cyberinfrastructure Contributors"). These people will likely need more advanced skills and some of them will become "Cyberinfrastructure Professionals" within our community. Section 5.7 has detailed our approach to scaling up software training activities to match the large size of the HL-LHC workforce.

The Training Grand Challenge defines a series of goals to guide our efforts. We consider the following three areas of impact:

- **Democratizing science with standardized prerequisites (done):** A series of standardized training modules covering all basic software prerequisites allows students to close any gaps in their knowledge before starting experiment onboarding.
- **Scaling up training for intermediate and advanced topics:** Regular intermediate- to advanced-level courses and workshops need to be organized and brought to the attention of both students and their supervisors. At the same time, all material should be self-study friendly and easily discoverable in a way that does not overwhelm students. To that end, our training center should be expanded to list all relevant and tested training resources across the field.
- **Establishing career paths for developers:** The career path toward cyberinfrastructure professionals or software-focused permanent positions must be firmly established. Specific workshops and mentoring opportunities for students focusing on software engineering skills need to be offered.

To achieve these goals in an efficient and sustainable fashion, we also define the following focus areas:

- **Building a community of educators:** We need to grow the community of cross-experiment educators that has been created by the IRIS-HEP/HSF Training group. This includes further improving the recognition and visibility of all contributors. Regular talks at major conferences and publications in journals such as the Journal of Open Source Education (JOSE) are important parts of this strategy. We should also expand our collaboration with experiments and similar initiatives focusing on open-source training, particularly the new initiatives centered around cyberinfrastructure for research.
- **Training material sustainability:** The community should firmly push to publish training material in editable and community-maintainable formats with open-source licenses. If traditional presentation software (PowerPoint, Keynote, Impress) is used, this means publishing corresponding editable files. However, the use of source file-based systems (e.g., presentations

built from LaTeX files, Markdown files, or Jupyter notebooks) should be encouraged. Workshops should encourage educators to follow these guidelines and, in particular, pay attention to licensing.

A series of milestones and an estimated timeline to achieve these goals is shown in Table 6.

Year	Target
2018 – 2022	• Develop and teach standardized training modules covering essential software prerequisites (completed). • Establish and grow a training group that coordinates and sustains cross-experiment training efforts (completed).
2023	• Seed topical subgroups that create new intermediate/advanced training material based on the State of Training 2022 survey. • Rebuild and expand the Training Center to become a focal point of *all* software training resources in HEP. • Strengthen collaborations with experiments and new organizations that support the career path of CI Professionals.
2024	The first intermediate-advanced training modules are being taught.
2025	• 80% of all cross-experiment software topics that apply to Ph.D. students should be covered by standardized training modules. • 90% of HEP Ph.D. students should be aware of the material offered by the IRIS-HEP/HSF Training group. • 50% of HEP Ph.D. students should participate in at least one intermediate/advanced training.
2026 - 2028	• Additional focus on workshops, networking opportunities, and discussion platforms for aspiring developers and CI professionals within HEP. • 20% of Ph.D. students and postdocs should be enrolled in software-related communities or have attended advanced workshops. • 20% of HEP Ph.D. students should teach or support a software workshop at one point during their Ph.D.

Table 6: Training activities and Training Grand Challenge goals to prepare the HL-LHC workforce.

7 Outreach and Broadening Participation

The participation of women and ethnic minorities is generally low in the HEP world, and fractionally it is even lower in the HEP Software and Computing (S&C) world. We estimate that fewer than 10% of people in HEP S&C are women while (from LHC experiment statistics) between 13% and 20% of the LHC experiments' collaborators are women. In the U.S., 7.4% of high-tech employment is black [73], while in HEP S&C the fraction is negligibly small. Other measures of HEP and HEP S&C diversity in the U.S. are likely to diverge in similar fashion from society at large. Looking forward, increasing the diversity of the HEP S&C workforce promises two types of benefits. From first principles, the top 5% of a larger pool should always be better than the top 10% of a pool half as large. In addition, studies show [74–76] that teams of people from diverse backgrounds are more innovative when crafting solutions to complex problems and can make better and more profitable decisions.

Minimally, IRIS-HEP must be (and is!) sensitive to diversity in building its own team, but that is not enough. Through its own directly-funded team IRIS-HEP alone cannot however significantly increase the fraction of under-represented populations in the larger HEP community or even in HEP S&C broadly. Even an NSF institute-class project like IRIS-HEP is too small a player by itself. What a project of this size can do, however, is help build the larger pipeline, and carefully align its efforts to be maximally effective by partnering with other institutions and projects actively working in the same direction.

In practice this means focusing on aspects of the program which engage people earlier in their academic careers. Most of the directly funded IRIS-HEP team is faculty, staff, postdocs or graduate students. At the high school level, IRIS-HEP has piloted at UPR-Mayagüez in Puerto Rico outreach activities with high school teachers around coding, machine learning and physics. By focusing on enabling teachers, we can multiply our impact. This is being expanded nationally via partnership with the QuarkNet [77] program which also engages high school teachers, including those connected with diverse groups of students. In particular IRIS-HEP has partnered post-COVID with QuarkNet in 2022 to develop a "Coding Camp 2" for high school teachers, which was piloted in summer 2022, at Fermilab. This adds to existing QuarkNet physics and software curriculum. In 2022-2023 we will leverage QuarkNet's existing national network of connections and local outreach programs at IRIS-HEP institutions to run 6 additional Coding Camp workshops for teachers in various locations. The overall aim is to reach nearly 100 high school teachers per year to help them develop basic software and physics-related training they can use in their classrooms. This program will continue in a second phase for IRIS-HEP.

At the undergraduate level, IRIS-HEP has developed an extensive training program (Section 5.7), including in particular a "Fellows" program which engages people in software-related physics research projects. This allows students to take general software skills they have learned and apply them to developing research software to solve problems in particle physics. Originally the Fellows program was focused on graduate students, however during COVID it evolved into a program that works primarily with undergraduate students. Each undergraduate Fellow works with a mentor on a (typically summer) research software project relevant for particle physics. Typically they work at a distance with their mentor, although some of the Fellows have traveled for a short period to work with their mentor in-person or to a conference or workshop.

Over the past couple of years IRIS-HEP has begun to align its training (Section 5.7 and Fellows mechanisms in ways that can also contribute to broadening participation. As noted earlier, student knowledge of basic software skills is very uneven. Experience with research software (and research activities in general) is less common at smaller and non-R1 institutions.

8 Funding Scenarios

In terms of scale, structure, and organization, the next phase of IRIS-HEP has a clear baseline for comparisons, namely the currently-funded institute. As outlined in Section 4, we envision that the basic concepts and organizational outlines of the institute as successful and thus would remain in place for the next phase. The large majority (approximately 90%) of the institute's funding goes to personnel; major non-personnel costs include the IRIS-HEP Fellows program, support for workshop, broader outreach activities, and one-time hardware purchases to bootstrap the Analysis Facilities activity. Table 2 shows that for IRIS-HEP year 5, about 90% of the personnel effort are in technical areas (either R&D or operations), 5% to training and outreach, and 5% to project management. While these precise splits will differ each year of the next phase, the approximate breakdowns are expected to remain.

In this strategic plan, three basic funding scenarios are considered: **low**, providing \$4 million per year, **medium**, providing \$5 million per year (the baseline level, the same as the current IRIS-HEP award), and **high**, providing \$6 million per year. In each scenario, we plan for five years of funding, supporting IRIS-HEP from the end of the first phase through the end of the research years running up to the HL-LHC.

In Section 5, each area has outlined a set of expected activities. The activities are further annotated to indicate the associated funding scenarios. For example, an activity marked as *medium scope (reduced activity), high* is expected to be fully supported in the high funding scenario, have a significantly reduced scope and scale in the medium funding scenario, and receive no support in the low funding scenario. Note the funding scenario labels to not necessarily correspond to *priority*; for example, in the DOMA area, the "Scaling the CI to HL-LHC data rates" is highest importance but, due to the effort required, would not be plausible in the low funding scenario (given this is key for the HL-LHC program as a whole, the Operations programs potentially would need to take on this activity). We do not attempt to rank the activities within each scenario; this level of detail is deferred for an actual project proposal.

A summary of each scenario is as follows:

- **Medium / Baseline Scenario**: In this scenario, which would most closely resemble the existing IRIS-HEP, with a scope encompassing the same activities as it does today. The Translational AI area (Section 5.3) would still be organized but it would be of modest size, approximately the same size as the aggregate exploratory AI R&D distributed throughout the institute areas. Areas would modestly evolve - for example, DOMA would still target adding the new XRootD activity at the cost of small reductions to other projects. The second phase of IRIS-HEP would slowly evolve from its current level of research today to focus more on development, deployment and sustainability towards the end of an 2nd 5-year mandate for the institute.
- **High Scenario**: In the high funding scenario, the new Translational AI area would be fully funded and expected to make a significant impact in the field. Other, more ambitious efforts in existing areas would be achievable – for example, the Analysis Systems would be able to make a realistic push toward completing the technologies required for a fully differentiable analysis in time for HL-LHC. The Reconstruction and Trigger Algorithms area would be able to directly support ML-based approaches to tracking and take larger risks in trying to close the resource gaps foreseen for HL-LHC. IRIS-HEP's second phase would have a larger mix of research activities throughout the project as it could support both research and sustainability activities simultaneously.
- **Low Scenario**: In this scenario, a 20% decrease to the budget from the current funding levels (a larger impact than 20% given the cumulative effects of inflation over the last five years),

IRIS-HEP would not start any new activities like XRootD or areas such as Translational AI. To meet funding levels, high-importance activities like the data grand challenge or entire areas such as Facilities R&D may need to be cut or combined into larger areas. The institute would pivot almost immediately to focus on completing and sustaining activities. Potentially, the institute would not be able to support any of the LHCb-related R&D activities.

A Appendix - Workshop List

One aspect of the Intellectual Hub role of IRIS-HEP is to help organize and coordinate community-wide meetings; this activity has been ongoing throughout the lifetime of the institute. During calendar year 2022, meetings IRIS-HEP was involved in or helped defined community needs and requirements include (in chronological order):

Analysis Ecosystems II Workshop
Date: 23–25 May 2022
Location: Laboratoire de Physique des 2 infinis Irène Joliot-Curie (Orsay, France)
URL: `https://indico.cern.ch/event/1125222/`
Summary report: `https://zenodo.org/record/7003962`
Description: (From workshop website) It has been five years since the first Analysis Ecosystems Workshop organised by the HSF in 2017. Since that time many changes have happened, with the advent of new projects, tools, and data formats, intense activity and progress in established projects. Still, the challenge of efficient analysis for the HL-LHC era is not yet solved and so the HSF and IRIS-HEP, together with IJCLab, are organising the Second Analysis Ecosystems Workshop.

Topics for the workshop include, amongst others:

- Analysis Facilities
- ML tools and differentiable computing workflows
- "Real-time" trigger-level analysis
- Analysis User Experience and Declarative Languages
- Analysis on reduced formats or specialist inputs
- Bookkeeping and systematics handling

Connecting the Dots 2022
Date: 31 May – 2 June 2022
Location: Princeton (Princeton, NJ)
URL: `https://indico.cern.ch/event/1103637/`
Description: (From workshop website) The Connecting The Dots workshop series brings together experts on track reconstruction and other problems involving pattern recognition in sparsely sampled data. While the main focus is on High Energy Physics (HEP) detectors, the Connecting The Dots workshop is intended to be inclusive across other scientific disciplines wherever similar problems or solutions arise.

Snowmass Community Summer Study Workshop
Date: 17 – 26 July 2022
Location: University of Washington (Seattle, WA)
URL: `http://seattlesnowmass2021.net/`
Description: (From workshop website) Snowmass21 is a yearlong study hosted by the Division of Particles and Fields (DPF) of the American Physical Society (APS), which takes place approximately every ten years. Its purpose is to define the most important questions for the field of particle physics and identify promising opportunities to address them. The study aims to be community-driven, inclusive, global, transparent, and interdisciplinary.

The Seattle meeting is the culmination of the various workshops and Town Hall meetings that have taken place during 2020, 2021, and 2022 as part of Snowmass21.

Second MODE Workshop on Differentiable Programming for Experiment Design

Date: 12 – 16 Sept 2022
Location: OAC conference center (Kolymbari, Crete, Greece)
URL: `https://indico.cern.ch/event/1145124/`
Description: The MODE (Machine-learning Optimized Design of Experiments) Collaboration aims to advance the idea of using differentiable programming for astro and particle physics. This workshop included invited keynote speakers, tutorials, and hackathons in the topic area and aims to coordinate the field's approach to differentiable programming.

PyHEP 2022 Workshop
Date: 12 – 16 September 2022
Location: (Virtual)
URL: `https://indico.cern.ch/event/1150631`
Description: (From workshop website) The PyHEP workshops are a series of workshops initiated and supported by the HEP Software Foundation (HSF) with the aim to provide an environment to discuss and promote the usage of Python in the HEP community at large.

IRIS-HEP Institute Retreat
Date: 12 – 14 October 2022
Location: Princeton (Princeton, NJ)
URL: `https://indico.cern.ch/event/1196111/`
Description: (From workshop website) The IRIS-HEP software institute has recently completed its fourth year after being funded by the National Science Foundation. The goals of the retreat were:

- Checkpoint the status of the IRIS-HEP efforts to date and specific plans and achievable goals for the next year (Year 5 of the project)
- Clarify the gaps between where we are now and what will be needed for the HL-LHC startup
- Elaborate a vision for what IRIS-HEP could do with an additional 5 year program of work

A Coordinated Ecosystem for HL-LHC Computing R&D
Date: 7 – 9 November 2022
Location: University of Notre Dame's Keough School of Global Affairs (Washington, DC)
URL: `https://indico.cern.ch/event/1203733`
Description: (From workshop website) The research and development efforts required to address the HEP challenges for the HL-LHC are challenging. The current LHC physics program is enabled by an elaborate software and computing ecosystem. The planned major hardware upgrades for the HL-LHC, and its planned physics program, will require significant evolution of this ecosystem. Major advances in software performance, adaptability, sustainability, workforce development and training that take full advantage of future data & compute platforms and leverage developments from outside of HEP are needed to succeed. Maintaining a coherent R&D effort in software and computing is required to achieve the physics goals of that era.

Software Citation and Recognition in HEP
Date: 22 – 23 November 2022
Location: (Virtual)
URL: `https://indico.cern.ch/event/1211229`
Description: (From workshop website) This meeting aims to provide a community discussion around ways in which HEP experiments handle citation of software and recognition for software efforts that enable physics results disseminated to the public.

B Appendix - Institute Organizational Structure and Evolutionary Process

The Institute's baseline organizational, management, and steering model is in Figure 17 and largely reflects the approach of IRIS-HEP. The specific choices may evolve in an eventual implementation phase depending on funding levels and project participants but the basic framework here is expected to be unchanged.

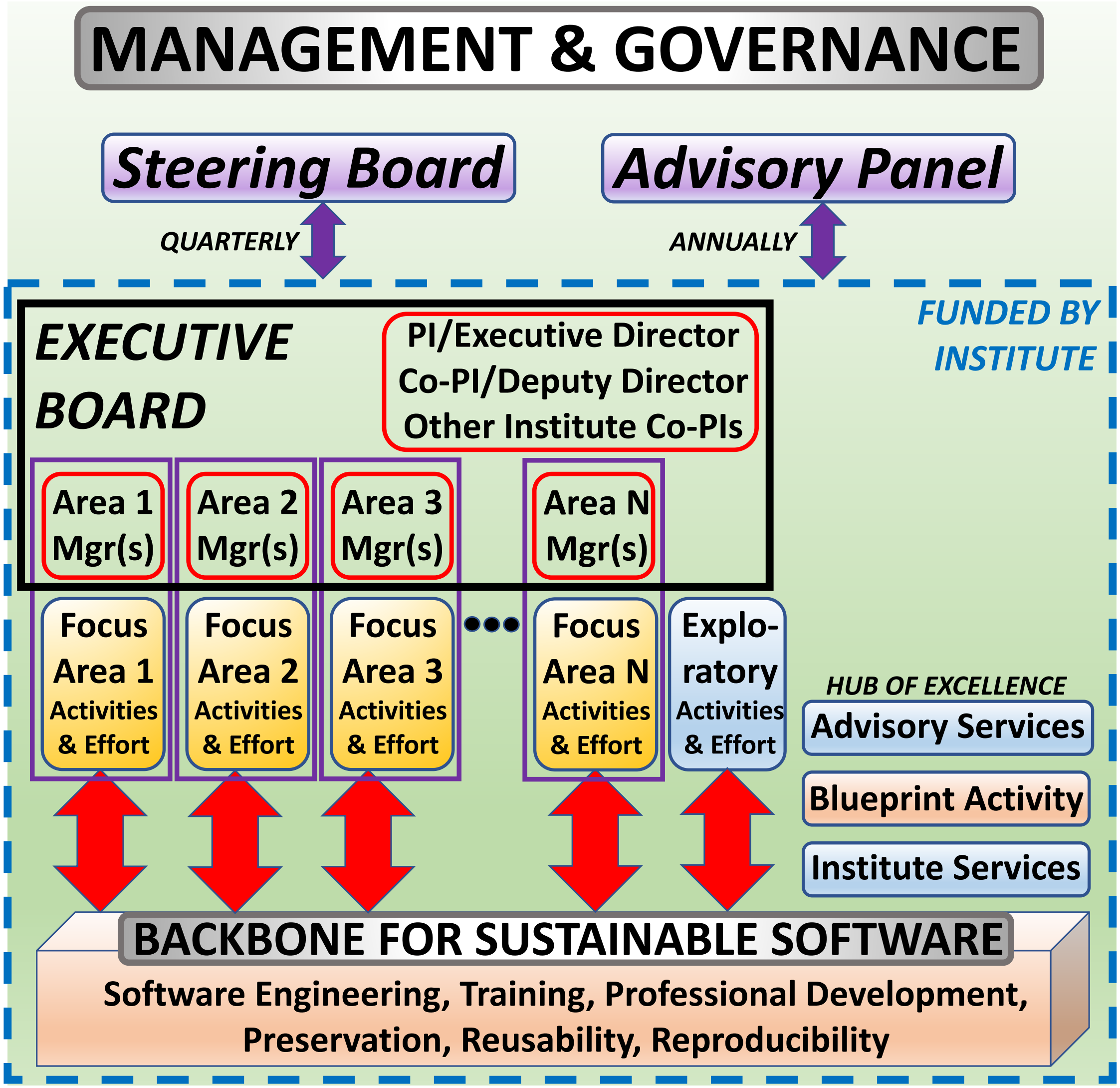

Figure 17: Baseline Model for Institute Management and Governance.

The main elements in this organizational structure and their roles within the Institute are:

PI/co-PIs: The PI/co-PIs on an eventual Institute implementation proposal will have project responsibilities as defined by NSF.

Focus Areas: A number of Focus Areas will be defined for the Institute at any given point in time. These areas will represent the main priorities of the Institute in terms of activities aimed at developing the software infrastructure to achieve the mission of the Institute. The initial set of strategic area are described in Section 5. The number and size of the areas ultimately included in the implementation will depend on the resources available to achieve the goals. The areas could evolve over the course of the Institute, but it is expected to be typically between six and eight. Each focus area within an Institute will have a written set of goals for the year and corresponding Institute resources as laid out in the project execution plan. The active focus areas will be reviewed once per year as part of the annual planning process and decisions will be taken on updating the list of areas and their yearly goals (with input from the Steering Board).

Area Manager(s): Each Area Manager will manage the day to day activities within a focus area. Special care will be taken to identify a deputy for each area to ensure continuity when a manager takes on a new position or role. An appropriate mix of HEP, Computer Science and representation from different experiments will be a goal when selecting the area managers.

Executive Board: The Executive Board will manage the day to day activities of the Institute. It will consist of the PI, co-PIs, and the area managers. A weekly meeting will be used to manage the general activities of the Institute and make shorter term plans. Liaisons from other organizations such as the U.S. LHC Ops programs would be invited as an “observer” to weekly Executive Board meetings in order to facilitate transparency and collaboration (e.g. on shared services or resources).

Steering Board: A Steering Board will be defined to meet with the executive board approximately quarterly to review the large scale priorities, strategy, and focus areas of the Institute. The steering board will consist of two representatives for each participating experiment, representatives of the U.S. LHC Operations programs, plus other representatives including CERN and FNAL. Members of the Steering Board will be proposed by their respective organizations and accepted by the Executive Director in consultation with the Executive Board.

Executive Director: An Executive Director will manage the overall activities of the Institute and its interactions with external entities. In general, day-to-day decisions will be taken by achieving consensus in the Executive Board and strategy and priority decisions based on advice and recommendations by the Steering and Executive Boards. In cases where consensus cannot be reached, the Executive Director will take a final decision. A Deputy Director will be included in the Institute organization, to assume duties of the Executive Director during periods of unavailability to ensure continuity of Institute operations.

Advisory Panel: An Advisory Panel will be convened to conduct an internal review of the project and future plans as needed. The members of the panel will be selected by the PI/co-PIs with input from the Steering Board. The panel will include experts not otherwise involved with the Institute in the areas of physics, computational physics, sustainable software development and cyberinfrastructure.

C Appendix - Glossary of Acronyms

ABC Approximate Bayesian Computation

ACAT A workshop series on Advanced Computing and Analysis Techniques in HEP.

ALICE A Large Ion Collider Experiment, an experiment at the LHC at CERN.

ALPGEN An event generator designed for the generation of Standard Model processes in hadronic collisions, with emphasis on final states with large jet multiplicities. It is based on the exact LO evaluation of partonic matrix elements, as well as top quark and gauge boson decays with helicity correlations.

AOD Analysis Object Data is a summary of the reconstructed event and contains sufficient information for common physics analyses.

ATLAS A Toroidal LHC ApparatuS, an experiment at the LHC at CERN.

BaBar A large HEP experiment which ran at SLAC from 1999 through 2008.

BSM Physics beyond the Standard Model (BSM) refers to the theoretical developments needed to explain the deficiencies of the Standard Model (SM), such as the origin of mass, the strong CP problem, neutrino oscillations, matter–antimatter asymmetry, and the nature of dark matter and dark energy.

CDN Content Delivery Network

CERN The European Laboratory for Particle Physics, the host laboratory for the LHC (and eventually HL-LHC) accelerators and the ALICE, ATLAS, CMS and LHCb experiments.

CHEP An international conference series on Computing in High Energy and Nuclear Physics.

CI Cyberinfrastructure, referring to the people, software, and hardware necessary that provide powerful and advanced capabilities

CMS Compact Muon Solenoid, an experiment at the LHC at CERN.

CMSSW Application software for the CMS experiment including the processing framework itself and components relevant for event reconstruction, high-level trigger, analysis, hardware trigger emulation, simulation, and visualization workflows.

CMSDAS The CMS Data Analysis School

CoDaS-HEP The COmputational and DAta Science in HEP school.

CP Charge and Parity conjugation symmetry

CPV CP violation

CS Computer Science

CRSG Computing Resources Scrutiny Group, a WLCG committee in charge of scrutinizing and assessing LHC experiment yearly resource requests to prepare funding agency decisions.

CTDR Computing Technical Design Report, a document written by one of the experiments to describe the experiment's technical blueprint for building the software and computing system

CVMFS The CERN Virtual Machine File System is a network file system based on HTTP and optimised to deliver experiment software in a fast, scalable, and reliable way through sophisticated caching strategies.

CVS Concurrent Versions System, a source code version control system

CWP The Community White Paper is the result of an organised effort to describe the community strategy and a roadmap for software and computing R&D in HEP for the 2020s. This activity is organised under the umbrella of the HSF.

DASPOS the Data And Software Preservation for Open Science project

Deep Learning one class of Machine Learning algorithms, based on a high number of neural network layers.

DES The Dark Energy Survey

DIANA-HEP the Data Intensive Analysis for High Energy Physics project, funded by NSF as part of the SI2 program

DOE The Department of Energy

DHTC Distributed High Throughput Computing

DOMA Data Organization, Management and Access, a term for an integrated view of all aspects of how a project interacts with and uses data.

EFT the Effective Field Theory, an extension of the Standard Model

EYETS Extended Year End Technical Stop, used to denote a period (typically several months) in the winter when small upgrades and maintenance are performed on the CERN accelerator complex and detectors

FNAL Fermi National Accelerator Laboratory, also known as Fermilab, the primary US High Energy Physics Laboratory, funded by the US Department of Energy

FPGA Field Programmable Gate Array

FTE Full Time Equivalent

FTS File Transfer Service

GAN Generative Adversarial Networks are a class of artificial intelligence algorithms used in unsupervised machine learning, implemented by a system of two neural networks contesting with each other in a zero-sum game framework.

GAUDI An event processing application framework developed by CERN

Geant4 A toolkit for the simulation of the passage of particles through matter.

GeantV An R&D project that aims to fully exploit the parallelism, which is increasingly offered by the new generations of CPUs, in the field of detector simulation.

GPGPU General-Purpose computing on Graphics Processing Units is the use of a Graphics Processing Unit (GPU), which typically handles computation only for computer graphics, to perform computation in applications traditionally handled by the Central Processing Unit (CPU). Programming for GPUs is typically more challenging, but can offer significant gains in arithmetic throughput.

HEP High Energy Physics

HEP-CCE the HEP Center for Computational Excellence, a DOE-funded cross-cutting initiative to promote excellence in high performance computing (HPC) including data-intensive applications, scientific simulations, and data movement and storage

HEPData The Durham High Energy Physics Database is an open access repository for scattering data from experimental particle physics.

HEPiX A series of twice-annual workshops which bring together IT staff and HEP personnel involved in HEP computing

HL-LHC The High Luminosity Large Hadron Collider is a proposed upgrade to the Large Hadron Collider to be made in 2026. The upgrade aims at increasing the luminosity of the machine by a factor of 10, up to $10^{35}\mathrm{cm}^{-2}\mathrm{s}^{-1}$, providing a better chance to see rare processes and improving statistically marginal measurements.

HLT High Level Trigger. Software trigger system generally using a large computing cluster located close to the detector. Events are processed in real-time (or within the latency defined by small buffers) and select those who must be stored for further processing offline.

HPC High Performance Computing.

HS06 HEP-wide benchmark for measuring CPU performance based on the SPEC2006 benchmark (https://www.spec.org).

HSF The HEP Software Foundation facilitates coordination and common efforts in high energy physics (HEP) software and computing internationally.

IgProf The Ignominius Profiler, a tool for exploring the CPU and memory use performance of very large C++ applications like those used in HEP

IML The Inter-experimental LHC Machine Learning (IML) Working Group is focused on the development of modern state-of-the art machine learning methods, techniques and practices for high-energy physics problems.

INFN The Istituto Nazionale di Fisica Nucleare, the main funding agency and series of laboratories involved in High Energy Physics research in Italy

JavaScript A high-level, dynamic, weakly typed, prototype-based, multi-paradigm, and interpreted programming language. Alongside HTML and CSS, JavaScript is one of the three core technologies of World Wide Web content production.

Jupyter Notebook This is a server-client application that allows editing and running notebook documents via a web browser. Notebooks are documents produced by the Jupyter Notebook App, which contain both computer code (e.g., python) and rich text elements (paragraph, equations, figures, links, etc...). Notebook documents are both human-readable documents containing the analysis description and the results (figures, tables, etc..) as well as executable documents which can be run to perform data analysis.

LEP The Large Electron-Positron Collider, the original accelerator which occupied the 27km circular tunnel at CERN now occupied by the Large Hadron Collider

LHC Large Hadron Collider, the main particle accelerator at CERN.

LHCb Large Hadron Collider beauty, an experiment at the LHC at CERN

LIGO The Laser Interferometer Gravitational-Wave Observatory

LS Long Shutdown, used to denote a period (typically 1 or more years) in which the LHC is not producing data and the CERN accelerator complex and detectors are being upgraded.

LSST The Large Synoptic Survey Telescope

ML Machine learning is a field of computer science that gives computers the ability to learn without being explicitly programmed. It focuses on prediction making through the use of computers and encompasses a lot of algorithm classes (boosted decision trees, neural networks. . .).

MREFC Major Research Equipment and Facilities Construction, an NSF mechanism for large construction projects

NAS The National Academy of Sciences

NCSA National Center of Supercomputing Applications, at the University of Illinois at Urbana-Champaign

NDN Named Data Networking

NSF The National Science Foundation

ONNX Open Neural Network Exchange, an evolving open-source standard for exchanging AI models

Openlab CERN openlab is a public-private partnership that accelerates the development of cutting-edge solutions for the worldwide LHC community and wider scientific research.

OSG The Open Science Grid

P5 The Particle Physics Project Prioritization Panel is a scientific advisory panel tasked with recommending plans for U.S. investment in particle physics research over the next ten years.

PI Principal Investigator

QA Quality Assurance

QC Quality Control

QCD Quantum Chromodynamics, the theory describing the strong interaction between quarks and gluons.

REANA REusable ANAlyses, a system to preserve and instantiate analysis workflows

REU Research Experience for Undergraduates, an NSF program to fund undergraduate participation in research projects

RRB Resources Review Board, a CERN committee made up of representatives of funding agencies participating in the LHC collaborations, the CERN management and the experiment's management.

ROOT A scientific software framework widely used in HEP data processing applications.

SciDAC Scientific Discovery through Advanced Computing, a DOE program to fund advanced R&D on computing topics relevant to the DOE Office of Science

SDSC San Diego Supercomputer Center, at the University of California at San Diego

SHERPA Sherpa is a Monte Carlo event generator for the Simulation of High-Energy Reactions of PArticles in lepton-lepton, lepton-photon, photon-photon, lepton-hadron and hadron-hadron collisions.

SIMD Single instruction, multiple data (**SIMD**), describes computers with multiple processing elements that perform the same operation on multiple data points simultaneously.

SI2 The Software Infrastructure for Sustained Innovation program at NSF

SKA The Square Kilometer Array

SLAC The Stanford Linear Accelerator Center, a laboratory funded by the US Department of Energy

SM The Standard Model is the name given in the 1970s to a theory of fundamental particles and how they interact. It is the currently dominant theory explaining the elementary particles and their dynamics.

SOW Statement of Work, a mechanism used to define the expected activities and deliverables of individuals funded from a subaward with a multi-institutional project. The SOW is typically revised annually, along with the corresponding budgets.

SSI The Software Sustainability Institute, an organization in the UK dedicated to fostering better, and more sustainable, software for research.

SWAN Service for Web based ANalysis is a platform for interactive data mining in the CERN cloud using the Jupyter notebook interface.

TMVA The Toolkit for Multivariate Data Analysis with ROOT is a standalone project that provides a ROOT-integrated machine learning environment for the processing and parallel evaluation of sophisticated multivariate classification techniques.

TPU Tensor Processing Unit, an application-specific integrated circuit by Google designed for use with Machine Learning applications

URSSI the US Software Sustainability Institute, an S^2I^2 conceptualization activity recommended for funding by NSF

WAN Wide Area Network

WLCG The Worldwide LHC Computing Grid project is a global collaboration of more than 170 computing centres in 42 countries, linking up national and international grid infrastructures. The mission of the WLCG project is to provide global computing resources to store, distribute and analyse data generated by the Large Hadron Collider (LHC) at CERN.

x86_64 64-bit version of the x86 instruction set, which originated wiht the Intel 8086, but has now been implemented on processors from a range of companies, including the Intel and AMD processors that make up the vast majority of computing resources used by HEP today.

XRootD Software framework that is a fully generic suite for fast, low latency and scalable data access.

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